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Physical Properties of Hydrocarbons

And Other Chemicals

VOLUME 4

R. W. GALLANT
CARL L. YAWS

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Physical Properties of Hydrocarbons

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VOLUME 4

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Physical Properties of Hydrocarbons
And Other Chemicals

VOLUME 4

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Physical Properties of Hydrocarbons

Volume 4

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CONTENTS

Chapter Page

1. C_5 TO C_7 NORMAL ALDEHYDES 1
2. C_8, C_{10} AND C_{12} NORMAL ALDEHYDES 14
3. C_5 TO C_7 NORMAL ACIDS 24
4. C_8, C_{10} AND C_{12} NORMAL ACIDS 34
5. C_{14}, C_{16} AND C_{18} NORMAL ACIDS 44
6. ADIPIC AND SUCCINIC ACIDS 54
7. C_8, C_{10} AND C_{12} NORMAL ALCOHOLS 64
8. C_{14}, C_{16} AND C_{18} NORMAL ALCOHOLS 74
9. C_5 KETONES 84
10. C_6 KETONES 94
11. C_5 ETHERS 104
12. C_1 TO C_3 FORMATES 114
13. C_4 FORMATES 124
14. C_3 ACETATES 134
15. C_4 ACETATES 144
16. C_4 GLYCOLS 154
17. C_6 GLYCOLS 164
18. PROPYLAMINES 174
19. DIAMINES 184
20. FORMAMIDES 194
21. ACETAMIDES 204
22. ACRYLONITRILE AND ADIPONITRILE 214

REFERENCES 224

Appendix

A. CONVERSION TABLES 230

B. COMPOUND INDEX BY FORMULA 231

C. COMPOUND INDEX BY NAME 237

PREFACE

The objective of this book is to provide the working engineer with all the essential data to design and run production facilities. The data are presented in graphs covering a wide temperature range to enable the engineer to quickly determine the information he needs at the desired temperature.

The literature has been carefully searched for experimental data. When several sources give different values, the authors made a judgment as to the most reliable source. To enable the engineer to go back to the original article for additional information, the sources of all data are documented.

For many compounds, experimental results are available only over a narrow temperature span. In these cases, estimation methods have been used to extend the data over a wider temperature range. When estimation methods are used, the method and expected accuracy are explained. Thus, the user is aware of the reliability of the graphical values. Reference to the original work is provided for those wishing to study the method further.

The physical properties normally needed in design and production are vapor pressure, heat of vaporization, density, surface tension, heat capacity and thermal conductivity. For chemical reactions, enthalpy of formation and Gibb's free energy of formation are helpful. Also, the boiling point, freezing point, molecular weight, critical properties, lower explosion limit in air and solubility in water are tabulated for each compound. This latter property data are helpful in safety and environmental engineering.

In this edition, special attention is paid to improving the accuracy of estimation techniques. Improved methods of extending data and new experimental data are included.

The SI and metric units are used for all properties except vapor pressure, both because these units are becoming increasingly used in production plants and because conversion is generally easier. Each graph displays a conversion factor providing English units. The temperature scale in all graphs is Centigrade.

Robert W. Gallant
Freeport, Texas

Carl L. Yaws
Beaumont, Texas

DISCLAIMER

This handbook presents a variety of thermodynamic and physical property data. It is incumbent upon the user to exercise judgment in the use of the data. The authors do not provide any guarantee, express or implied, with regard to the general or specific applicability of the data, the range of errors that may be associated with any of the data, or the appropriateness of using any of the data in any subsequent calculation, design or decision process. The authors accepts no responsibility for damages, if any, suffered by any reader or user of this handbook as a result of decisions made or actions taken on information contained herein.

CONTRIBUTORS

Li Bu	Graduate Student, Chemical Engineering Department, Lamar University, Beaumont, Texas 77710, U S A
Robert W. Gallant	Vice President and Director, North America Operations, Dow Chemical Company, Midland, Michigan 48674, U S A
Xiaoyan Lin	Graduate Student, Chemical Engineering Department, Lamar University, Beaumont, Texas 77710, U S A
Carl L. Yaws	Professor, Chemical Engineering Department, Lamar University, Beaumont, Texas 77710, U S A

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Carl L. Yaws

Physical Properties of Hydrocarbons

And Other Chemicals

VOLUME 4

Chapter 1

C_5 TO C_7 NORMAL ALDEHYDES

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 1-1

Physical, thermodynamic and transport property data from the literature (2,3,36-38,44-60,62-71) are given in Table 1-1. The critical constants are from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available. Results from the DIPPR (Design Institute for Physical Property Research) project (5) and recent data compilations by Yaws and co-workers (44-60) were consulted extensively in preparing the tabulation.

The property data in the top and middle parts of the tabulation are helpful in process engineering. The property data in the lower part of the tabulation are helpful in safety and environmental engineering.

VAPOR PRESSURE - Figure 1-1

Results from the DIPPR project (5) were selected. These results are applicable for vapor pressure from very low temperatures to the critical point. Correlation of vapor pressure as a function of temperature was accomplished using the equation:

$$\ln P = A + B/T + C \ln T + D\, T^{E} \tag{1-1}$$

where P = vapor pressure
T = temperature

Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 3% or less in most cases.

HEAT OF VAPORIZATION - Figure 1-2

Results from the DIPPR project (5) were selected. Data for heat of vaporization were correlated using a modified Watson equation with extended terms in the exponent:

$$\Delta H_{vap} = A\,(1 - T_r)^{[B + C\,T_r + D\,T_r^2 + E\,T_r^3]} \tag{1-2}$$

where ΔH_{vap} = heat of vaporization
T_r = reduced temperature, T/T_C

Reliability of results is good with errors of about 5% or less.

For data compilation of Yaws and co-workers (44,54), data for heat of vaporization were correlated using the Watson equation:

$$\Delta H_{vap} = A\ (1 - T_r)^{0.38} \tag{1-2a}$$

LIQUID DENSITY - Figure 1-3

Results from the DIPPR project (5) were selected. A modified Rackett equation was used for correlation of the data:

$$\rho = A\ B^{-(1 - T/C)^D} \tag{1-3}$$

where ρ = saturated liquid density
T = temperature

Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

For data compilation of Yaws and co-workers (44,54), a slightly different Rackett equation was used for correlation of the data:

$$\rho = A\ B^{-(1 - T_r)^{2/7}} \tag{1-3a}$$

where T_r = reduced temperature, T/T_C

SURFACE TENSION - Figure 1-4

Results from the DIPPR project (5) were selected. Using data from the literature, surface tension over the full liquid range was achieved by the modified Othmer equation:

$$\sigma = A\ (1 - T_r)^{[B + C\ T_r + D\ T_r^2 + E\ T_r^3]} \tag{1-4}$$

where σ = surface tension
T_r = reduced temperature, T/T_C

Accuracy is good with errors being about 5% or less in most cases.

For data compilation of Yaws and co-workers (44,54), surface tension was correlated by a slightly different Othmer equation:

$$\sigma = A\ (1 - T_r)^{11/9} \tag{1-4a}$$

HEAT CAPACITY - Figures 1-5 and 1-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Two different equations were used for correlation of the data for heat capacity of ideal gas:

$$C_P = A + B \exp\ [-C/T^D] \tag{1-5}$$

$$C_P = A + B\,[(C/T)/\sinh(C/T)]^2 + D\,[(E/T)/\cosh(E/T)]^2 \qquad (1\text{-}5a)$$

where C_P = heat capacity of ideal gas
T = temperature

Results are in favorable agreement with data. Errors are about 1% or less in most cases.

For data compilation of Yaws and co-workers (44,54), Correlation of data was accomplished using a series expansion in temperature:

$$C_P = A + B\,T + C\,T^2 + D\,T^3 \qquad (1\text{-}5b)$$

Results from the DIPPR project (5) were selected for heat capacity of liquid. Data were correlated with a series expansion in temperature:

$$C_P = A + B\,T + C\,T^2 + D\,T^3 + E\,T^4 \qquad (1\text{-}6)$$

where C_P = heat capacity of liquid
T = temperature

Results are in favorable agreement with data. Errors are about 10% or less using the equation. To provide wider coverage, the temperature range was extended using thermodynamic principles.

For data compilation of Yaws and co-workers (44,54), the following equation was used for heat capacity of liquid:

$$C_P = A + B\,T + C\,T^2 \qquad (1\text{-}6a)$$

VISCOSITY - Figures 1-7 and 1-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data were correlated using the equation:

$$\eta_{gas} = \frac{A\,T^B}{1 + C/T + D/T^2} \qquad (1\text{-}7)$$

where η_{gas} = viscosity of gas
T = temperature

Results are in favorable agreement with data. Errors are about 10% or less in most cases.

For the data compilation of Yaws and co-workers (31), a series expansion in temperature was used for viscosity of gas:

$$\eta_{gas} = A + B\,T + C\,T^2 \qquad (1\text{-}7a)$$

Results from the DIPPR project (5) were selected for viscosity of liquid. Data were correlated using the de Guzman - Andrade equation with extended terms:

$$\ln \eta_{liq} = A + B/T + C \ln T + D T^E \quad (1\text{-}8)$$

where η_{liq} = viscosity of liquid
T = temperature

Correlation results and data are in fair agreement with errors being about 10% or less.

For the data compilation of Yaws and co-workers (31), a modified de Guzman - Andrade equation was used for viscosity of liquid:

$$\log \eta_{liq} = A + B/T + C T + D T^2 \quad (1\text{-}8a)$$

THERMAL CONDUCTIVITY - Figures 1-9 and 1-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data were correlated using the equation:

$$\lambda_{gas} = \frac{A T^B}{1 + C/T + D/T^2} \quad (1\text{-}9)$$

where λ_{gas} = thermal conductivity of gas
T = temperature

Reliability of results is good with errors of about 10% or less in most cases.

For the data compilation of Yaws and co-workers (31), a series expansion in temperature was used for thermal conductivity of gas:

$$\lambda_{gas} = A + B T + C T^2 + D T^3 \quad (1\text{-}9a)$$

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. Data were correlated using the equation:

$$\lambda_{liq} = A + B T + C T^2 + D T^3 + E T^4 \quad (1\text{-}10)$$

where λ_{liq} = thermal conductivity of liquid
T = temperature

Results are in favorable agreement with data. Errors are about 5% or less in most cases.

For the data compilation of Yaws and co-workers (31), a series expansion with less terms was used for thermal conductivity of liquid:

$$\lambda_{liq} = A + B T + C T^2 \quad (1\text{-}10a)$$

ENTHALPY OF FORMATION - Figure 1-11

Results from the data compilation of Yaws and co-workers (44,45) were selected. The correlation for enthalpy of formation of the ideal gas is a series expansion in temperature:

$$\Delta H_f = A + B\,T + C\,T^2 \tag{1-11}$$

where ΔH_f = enthalpy of formation of ideal gas
T = temperature

Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 1-12

Results from the data compilation of Yaws and co-workers (44,46) were selected. The correlation for Gibb's free energy of formation of the ideal gas is a series expansion in temperature:

$$\Delta G_f = A + B\,T + C\,T^2 \tag{1-12}$$

where ΔH_f = Gibb's free energy of formation of the ideal gas
T = temperature

Results from the correlation are in favorable agreement with data.

CORRELATION CONSTANTS FOR EQUATIONS

The A, B, C, D and E in the above equations are correlation constants for the specific property under discussion. The correlation constants which have distinct values for individual compounds maybe used in the above equations to calculate the specific property value at the temperature of interest.

Table 1-1 Physical Properties

1. Name	Pentanal	Hexanal	Heptanal
2. Formula	C5H10O	C6H12O	C7H14O
3. Molecular Weight, g/mol	86.134	100.161	114.188
4. Critical Temperature, K	554.00	579.00	603.00
5. Critical Pressure, bar	35.000	31.100	28.000
6. Critical Volume, ml/mol	316.00	369.00	421.00
7. Critical Compressibility Factor	0.240	0.238	0.235
8. Acentric Factor	0.3931	0.4390	0.4865
9. Melting Point, K	182.00	217.15	230.15
10. Boiling Point @ 1 atm, K	376.15	401.45	425.95
11. Heat of Vaporization @ BP, kJ/kg	400.31	364.83	339.79
12. Density of Liquid @ 25 C, g/ml	0.805	0.810	0.813
13. Surface Tension @ 25 C, dynes/cm	24.98	25.97	26.26
14. Heat Capacity of Gas @ 25 C, J/g K	1.453	1.483	1.499
15. Heat Capacity of Liquid @ 25 C, J/g K	2.102	2.006	2.194
16. Viscosity of Gas @ 25 C, micropoise	65.285	60.976	57.552
17. Viscosity of Liquid @ 25 C, centipoise	0.614	0.780	0.953
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.010	0.010	0.009
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.138	0.137	0.137
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-227.93	-248.42	-264.17
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-108.61	-100.51	-87.12
22. Flash Point, K	285.15	299.82	310.93
23. Autoignition Temperture, K	495.15	------	------
24. Lower Explosion Limit in Air, vol %	1.5	1.3	1.1
25. Upper Explosion Limit in Air, vol %	9.50	8.10	7.1
26. Solubility in Water @ 30 C, ppm(wt)	22,030	5,644	1,516

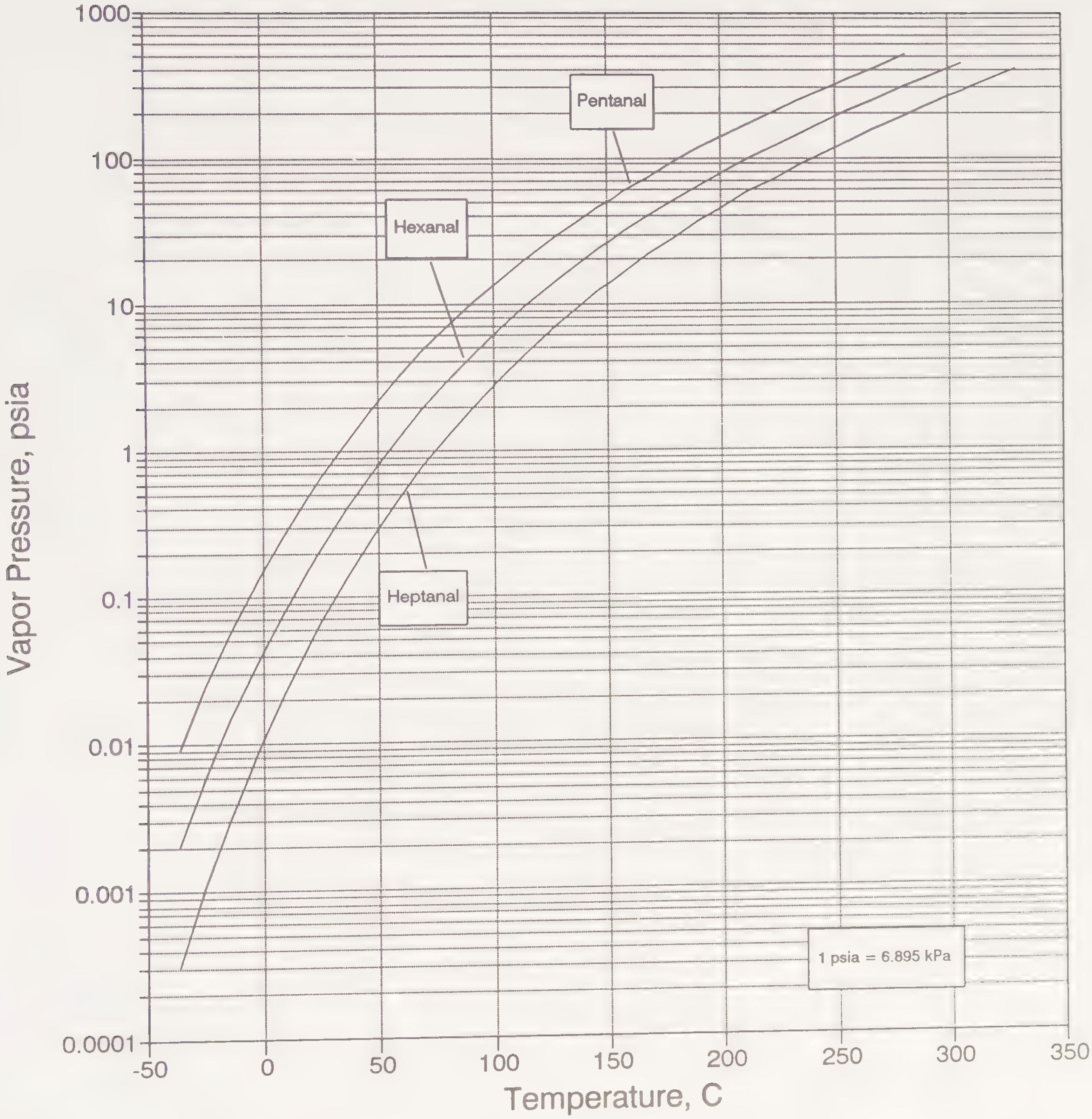

Figure 1-1 Vapor Pressure

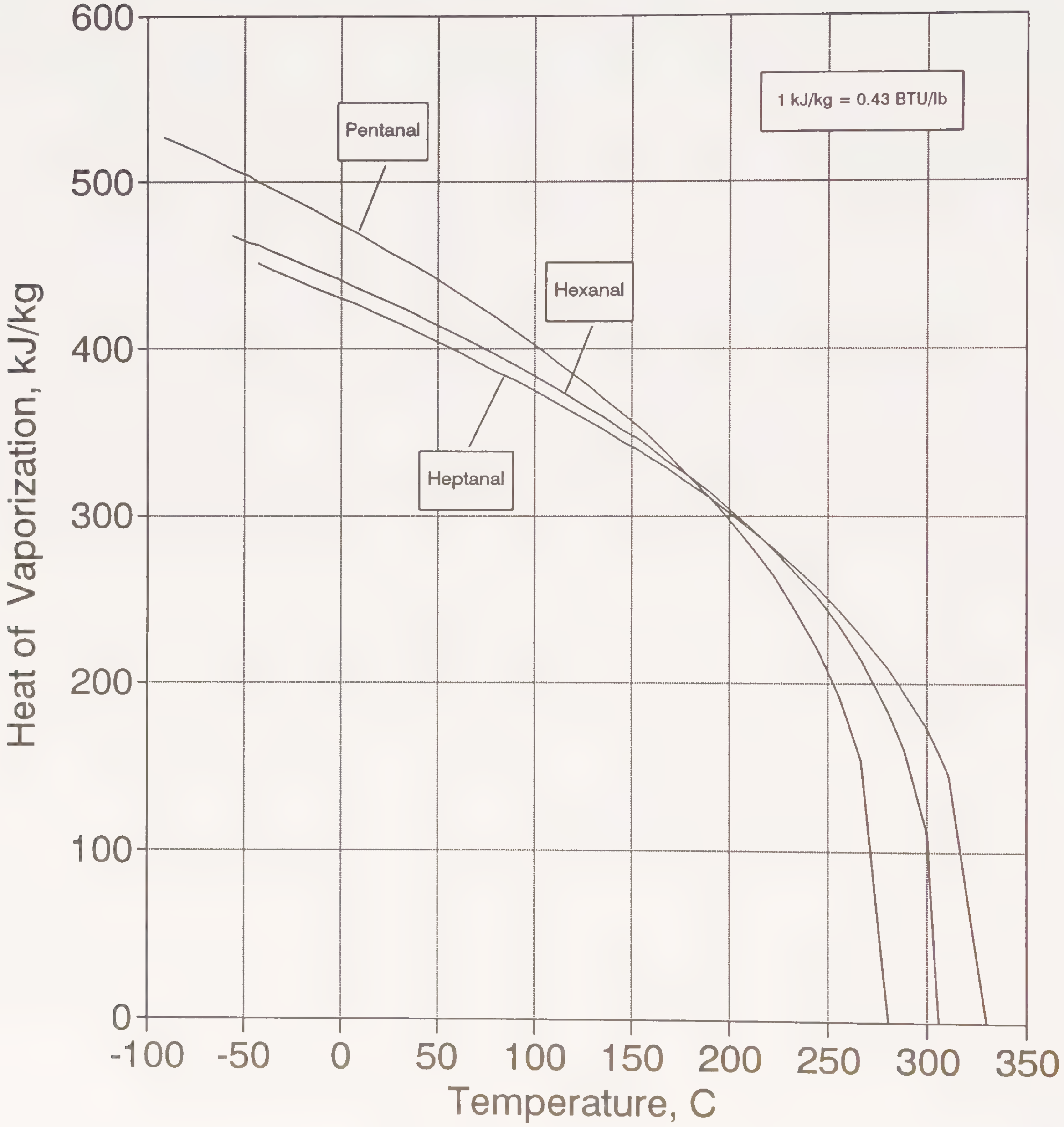

Figure 1-2 Heat of Vaporization

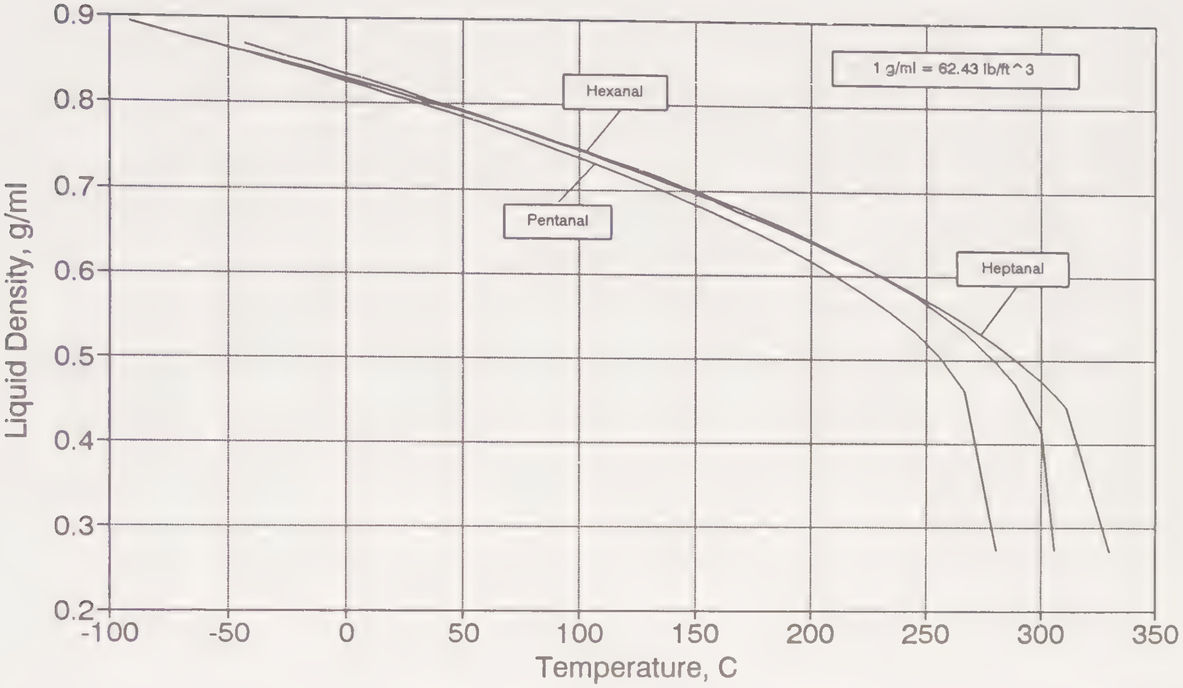

Figure 1-3 Liquid Density

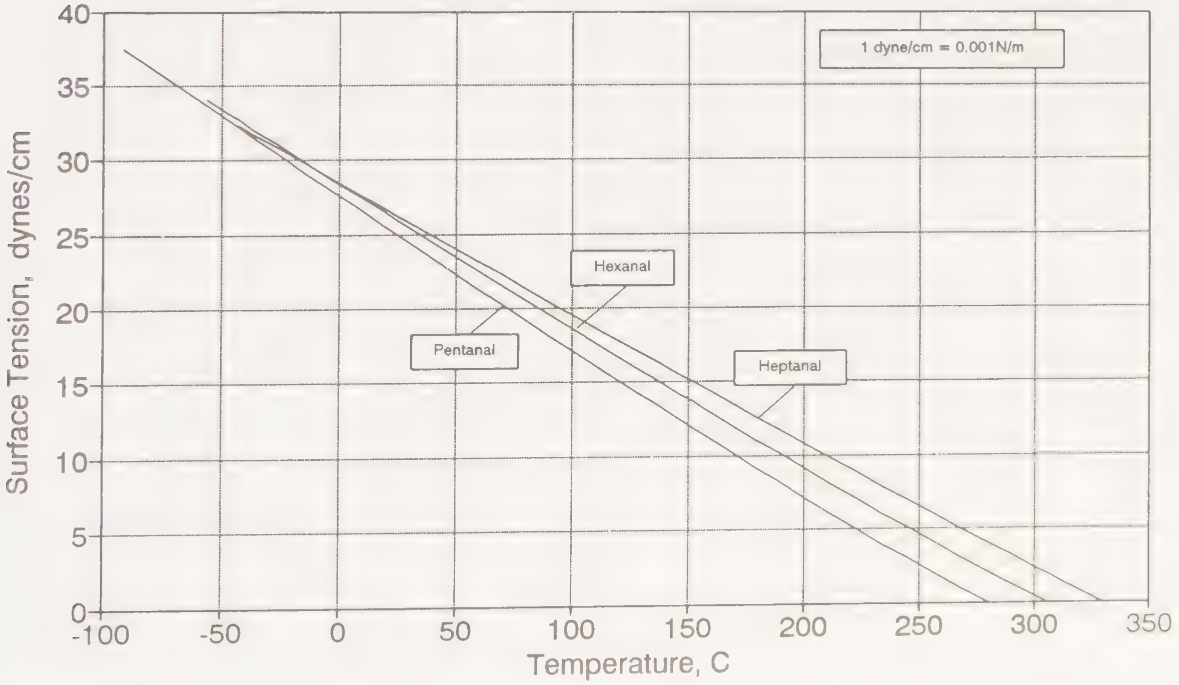

Figure 1-4 Surface Tension

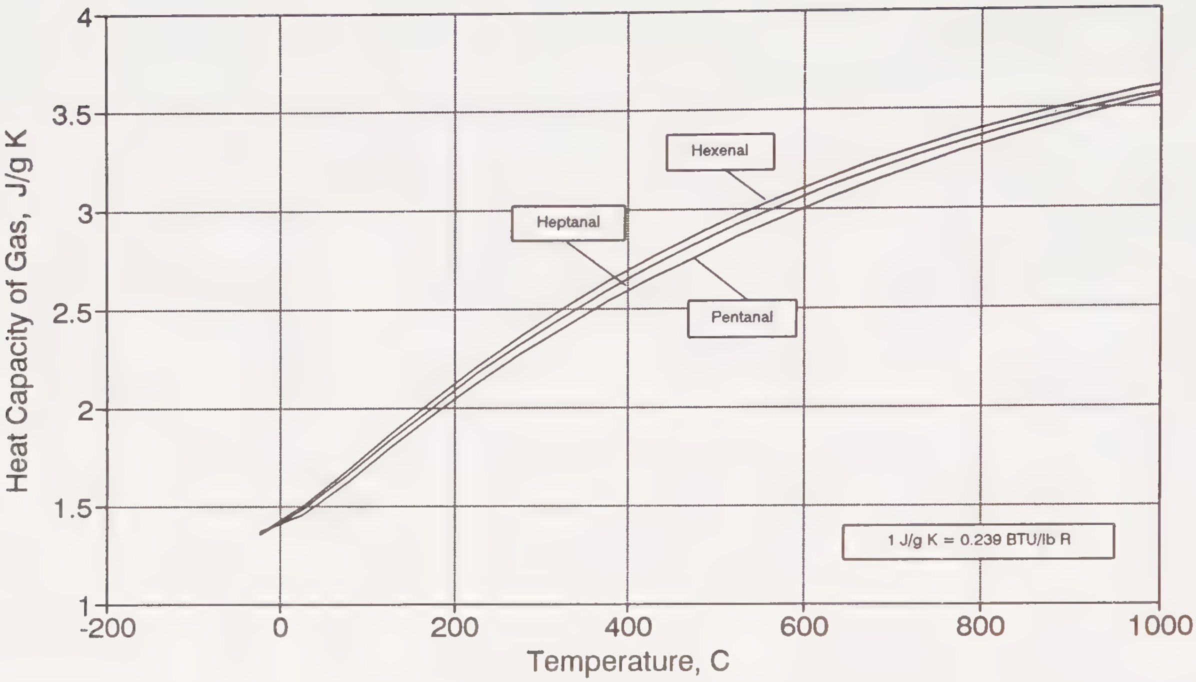

Figure 1-5 Heat Capacity of Gas

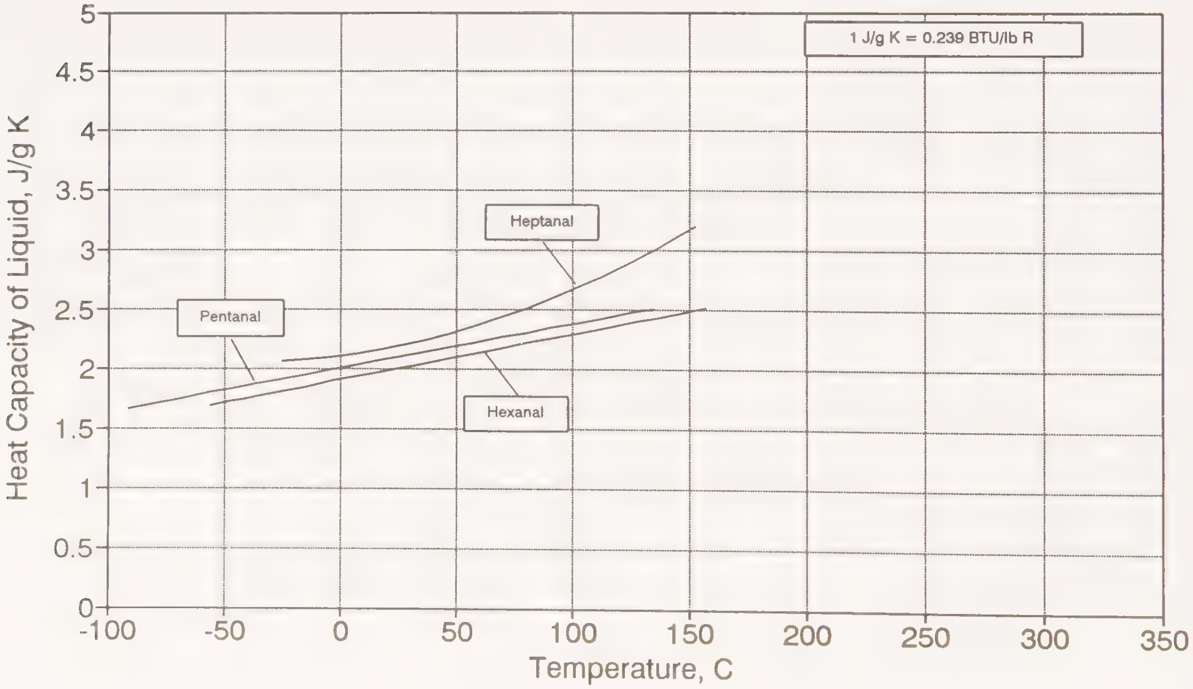

Figure 1-6 Heat Capacity of Liquid

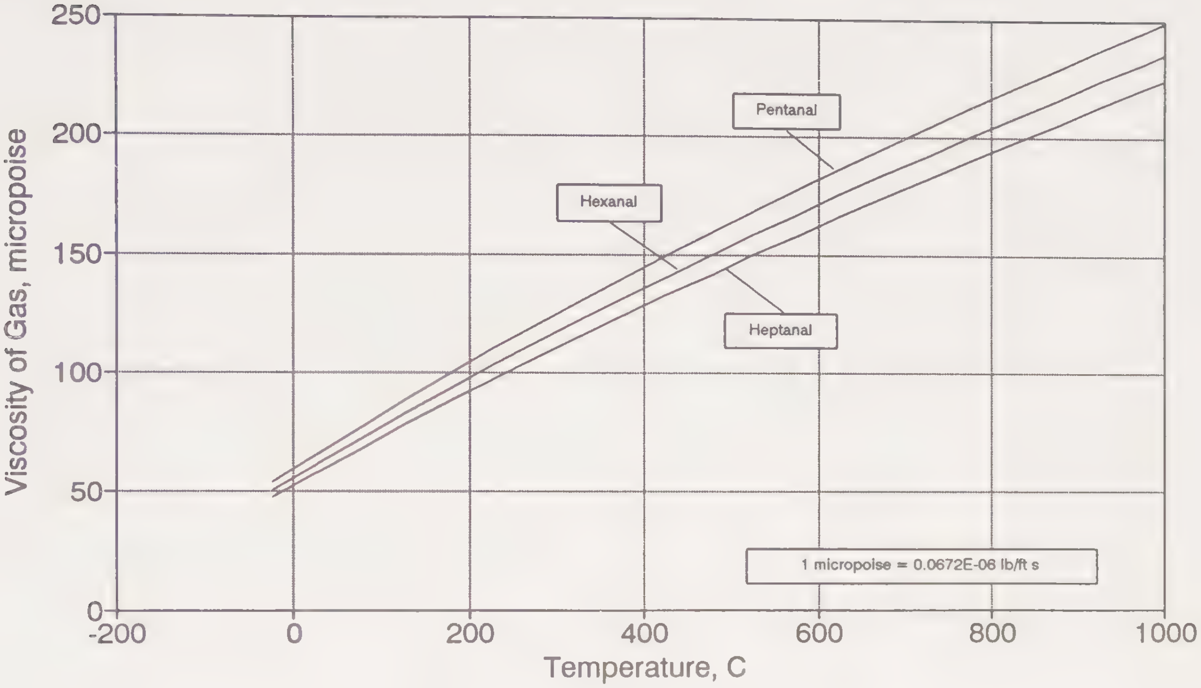

Figure 1-7 Viscosity of Gas

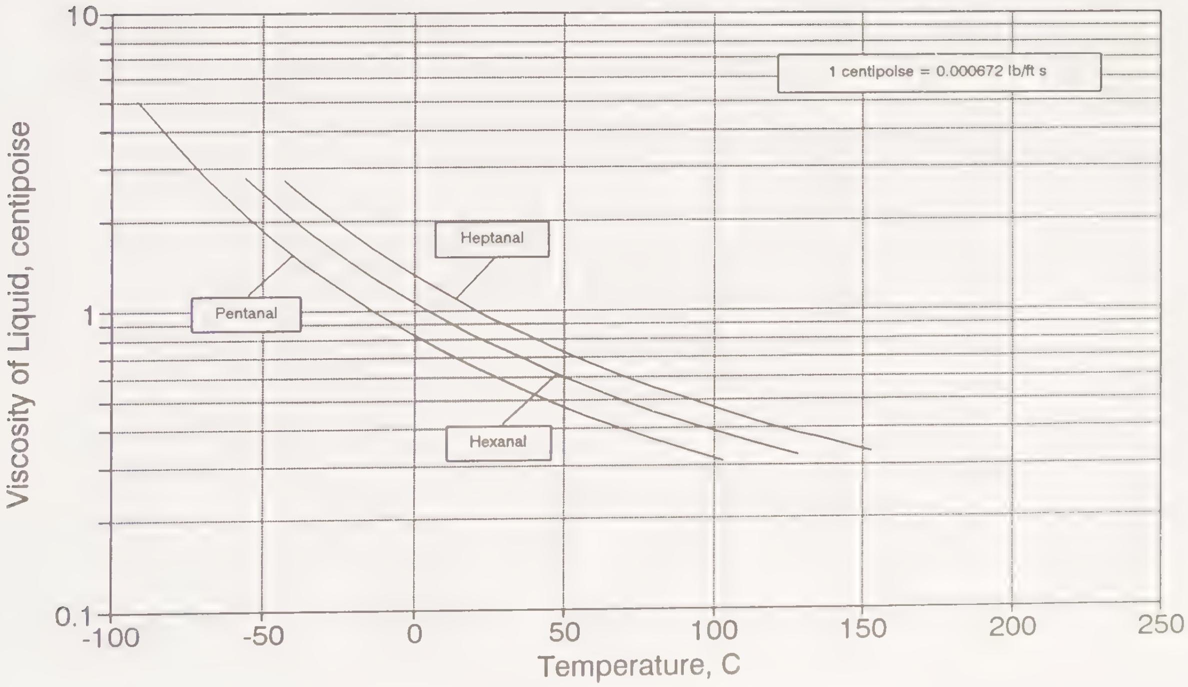

Figure 1-8 Viscosity of Liquid

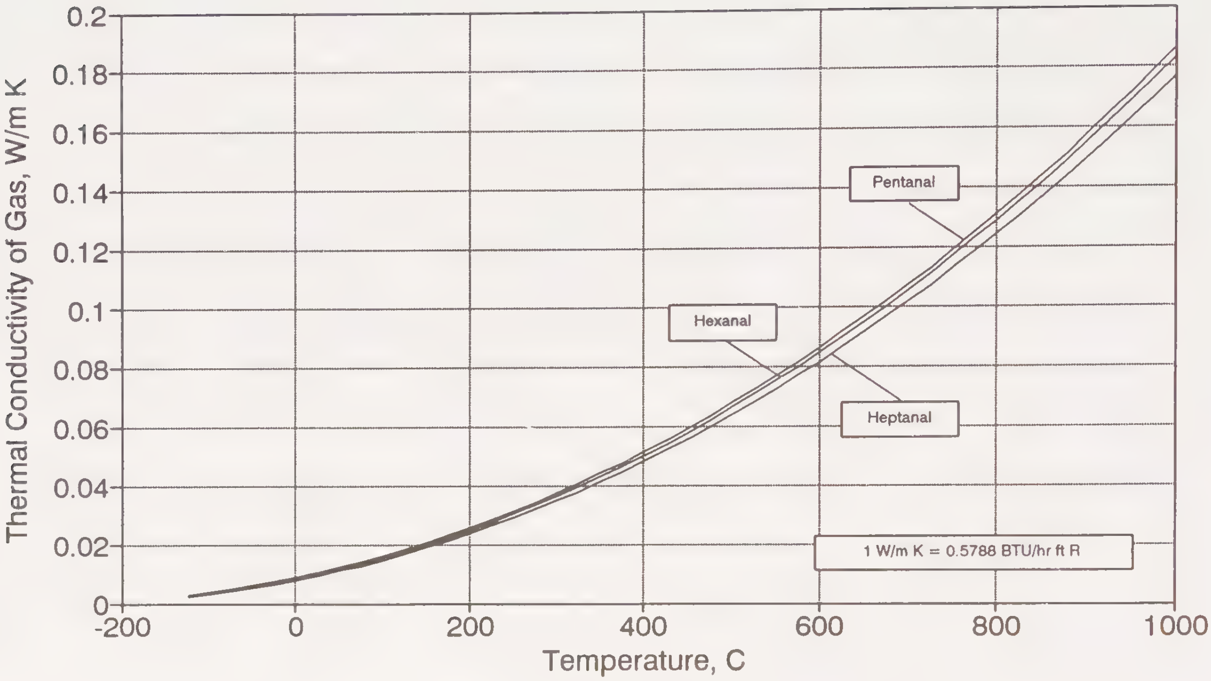

Figure 1-9 Thermal Conductivity of Gas

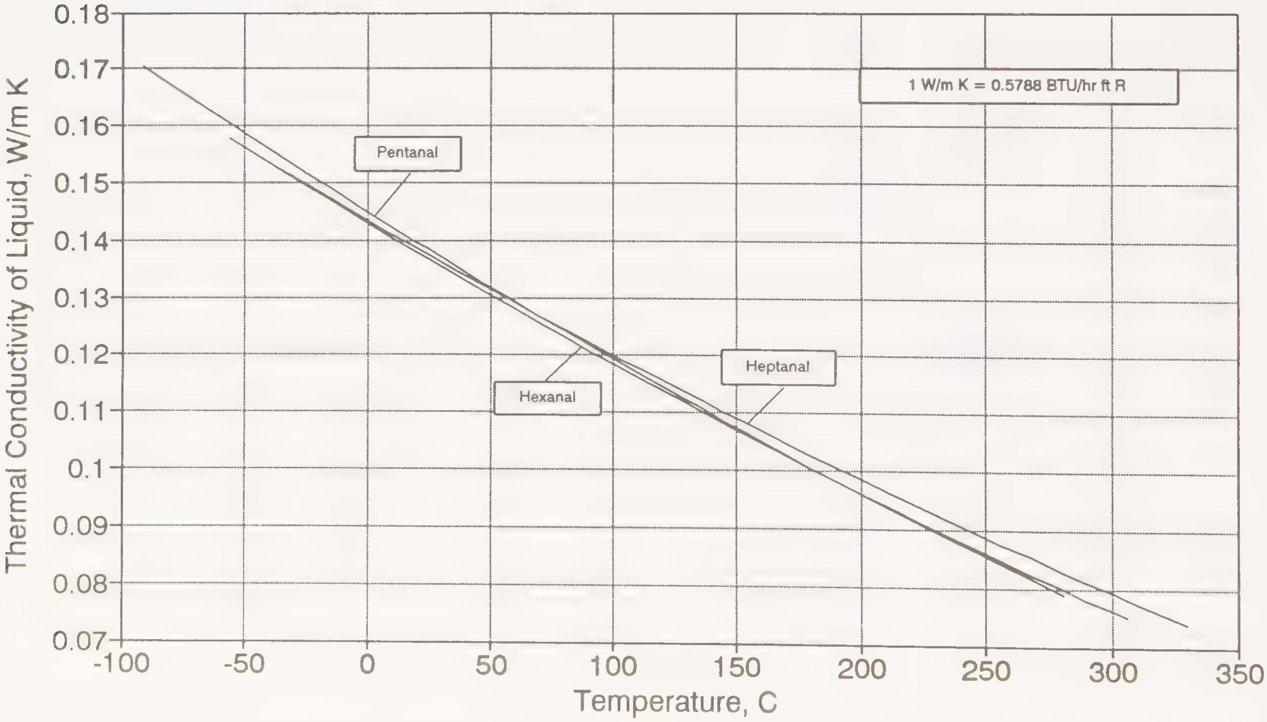

Figure 1-10 Thermal Conductivity of Liquid

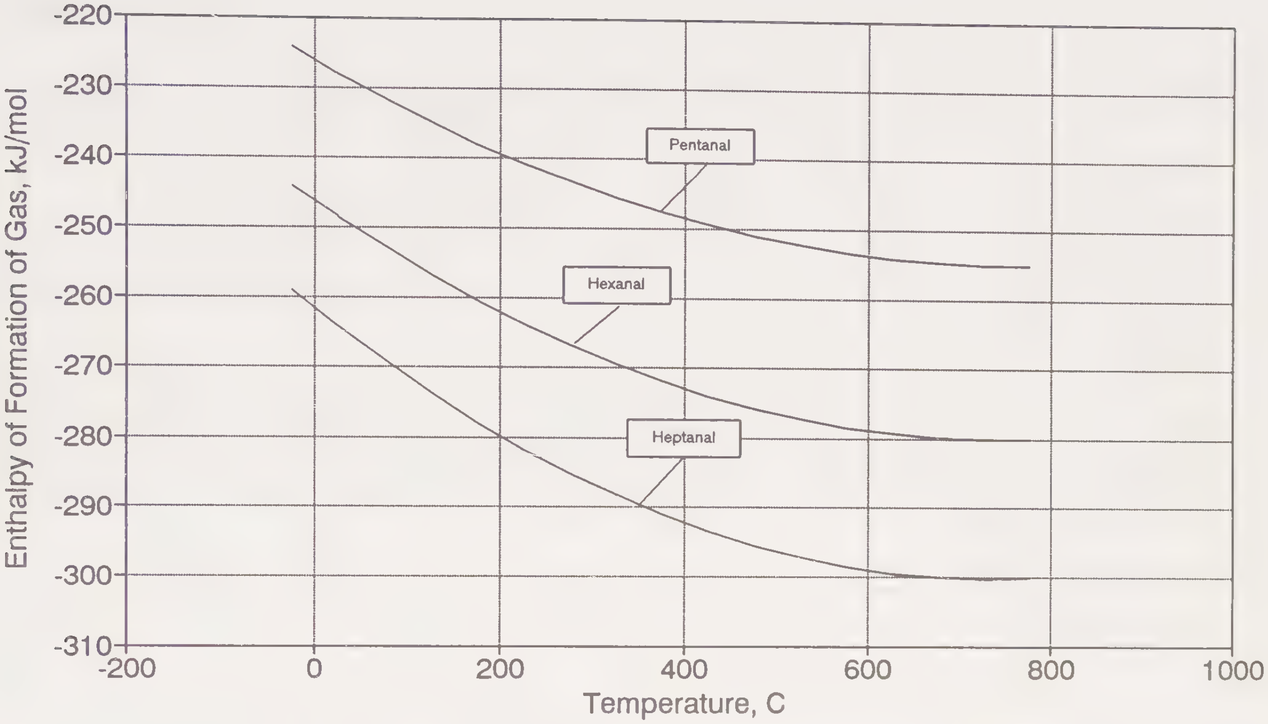

Figure 1-11 Enthalpy of Formation of Gas

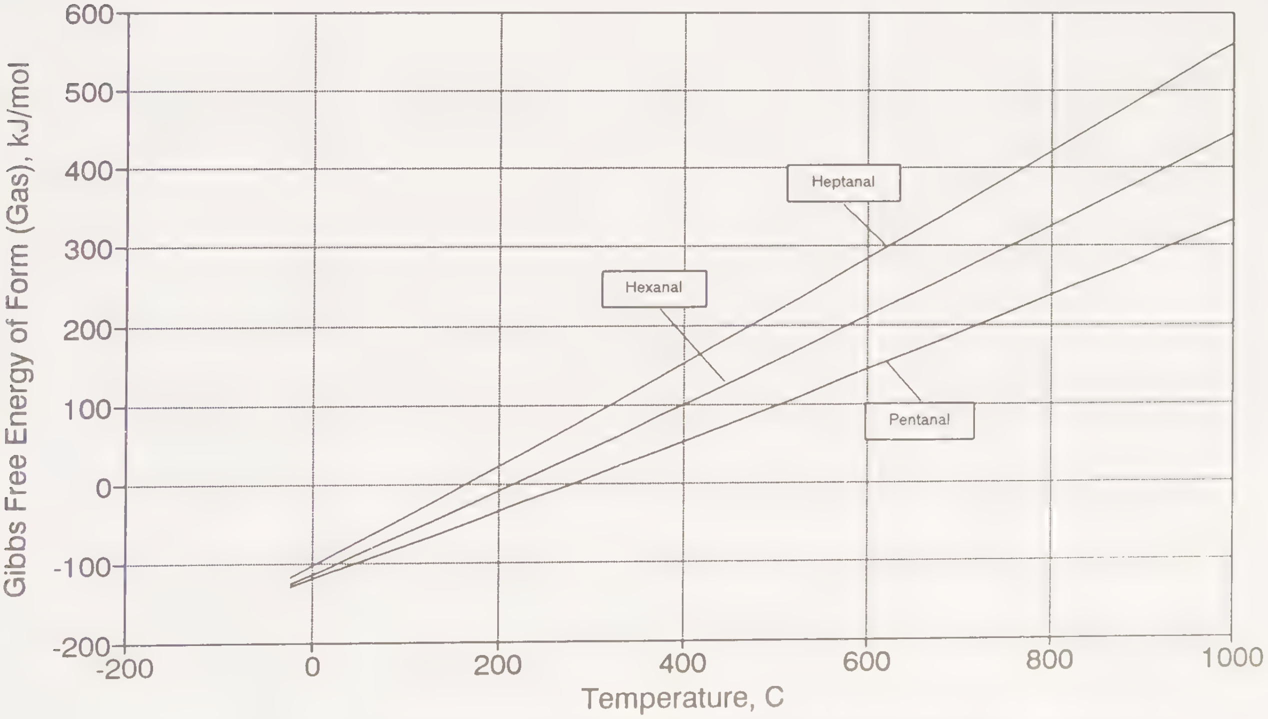

Figure 1-12 Gibbs Free Energy of Formation of Gas

Chapter 2

C_8, C_{10} AND C_{12} NORMAL ALDEHYDES

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 2-1

Property data from the literature (2,3,4,63-68,71-76) are given in Table 2-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available. The DIPPR (Design Institute for Physical Property Research) project (5) and data compilations by Yaws and co-workers (44) were consulted extensively in preparing the tabulation.

VAPOR PRESSURE - Figure 2-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 3% or less in most cases.

HEAT OF VAPORIZATION - Figure 2-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 5%.

LIQUID DENSITY - Figure 2-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 5% in most cases.

SURFACE TENSION - Figure 2-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 2-5 and 2-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 3% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 10% or less in most cases.

VISCOSITY - Figures 2-7 and 2-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 10% or less in most cases.

THERMAL CONDUCTIVITY - Figures 2-9 and 2-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is fair with possible errors of 10%.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 5% in most case except octanal(possible 25% error).

ENTHALPY OF FORMATION - Figure 2-11

The data compilation of Yaws and co-workers (44,45) was selected for enthalpy of formation of ideal gas for all component except dodecanal. For dodecanal, the values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 2-12

The data compilation of Yaws and co-workers (44,45) was selected for Gibb's free energy of formation of ideal gas for all component except dodecanal. For dodecanal, the values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 2-1 Physical Properties

1. Name	Octanal	Decanal	Dodecanal
2. Formula	C8H16O	C10H20O	C12H24O
3. Molecular Weight, g/mol	128.214	156.268	184.322
4. Critical Temperature, K	621.00	657.00	685.00
5. Critical Pressure, bar	25.500	21.500	18.600
6. Critical Volume, ml/mol	474.00	580.00	685.00
7. Critical Compressibility Factor	0.234	0.228	0.224
8. Acentric Factor	0.5471	0.6416	0.7538
9. Melting Point, K	246.00	267.15	285.15
10. Boiling Point @ 1 atm, K	447.15	488.15	523.15
11. Heat of Vaporization @ BP, kJ/kg	327.01	299.02	273.14
12. Density of Liquid @ 25 C, g/ml	0.816	0.821	0.826
13. Surface Tension @ 25 C, dynes/cm	27.33	28.11	28.67
14. Heat Capacity of Gas @ 25 C, J/g K	1.510	1.590	1.556
15. Heat Capacity of Liquid @ 25 C, J/g K	1.973	1.991	2.199
16. Viscosity of Gas @ 25 C, micropoise	55.38	49.30	44.91
17. Viscosity of Liquid @ 25 C, centipoise	1.150	1.542	1.910
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.009	0.008	0.007
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.130	0.144	0.154
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-289.95	-331.15	-375.51
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-83.84	-67.17	-55.31
22. Flash Point, K	325.00	358.15	378.00
23. Autoignition Temperture, K	------	------	------
24. Lower Explosion Limit in Air, vol %	1.0	0.8	0.6
25. Upper Explosion Limit in Air, vol %	6.4	5.4	5.0
26. Solubility in Water @ 25 C, ppm(wt)	370.3 @ 30 C	------	------

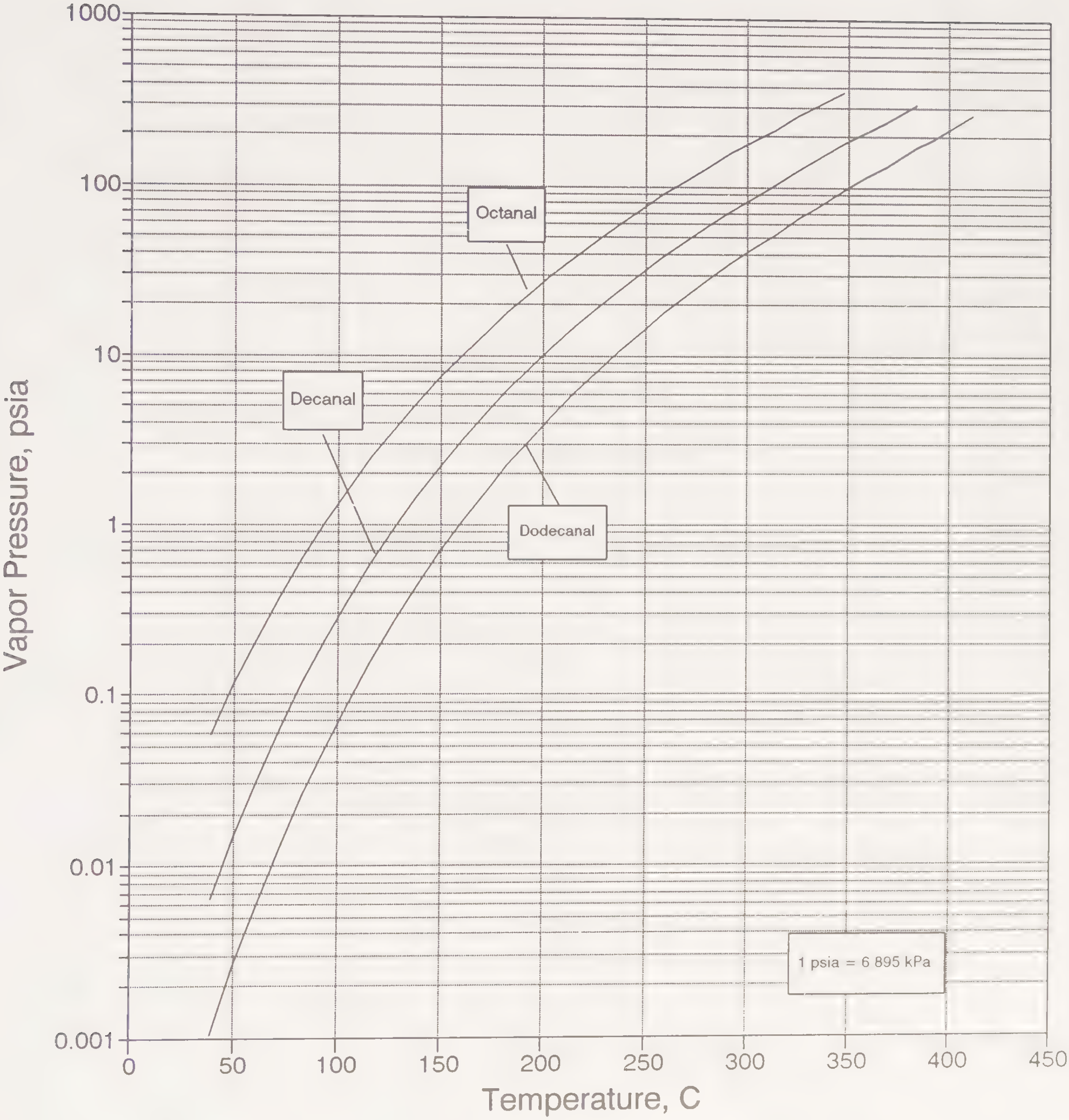

Figure 2-1 Vapor Pressure

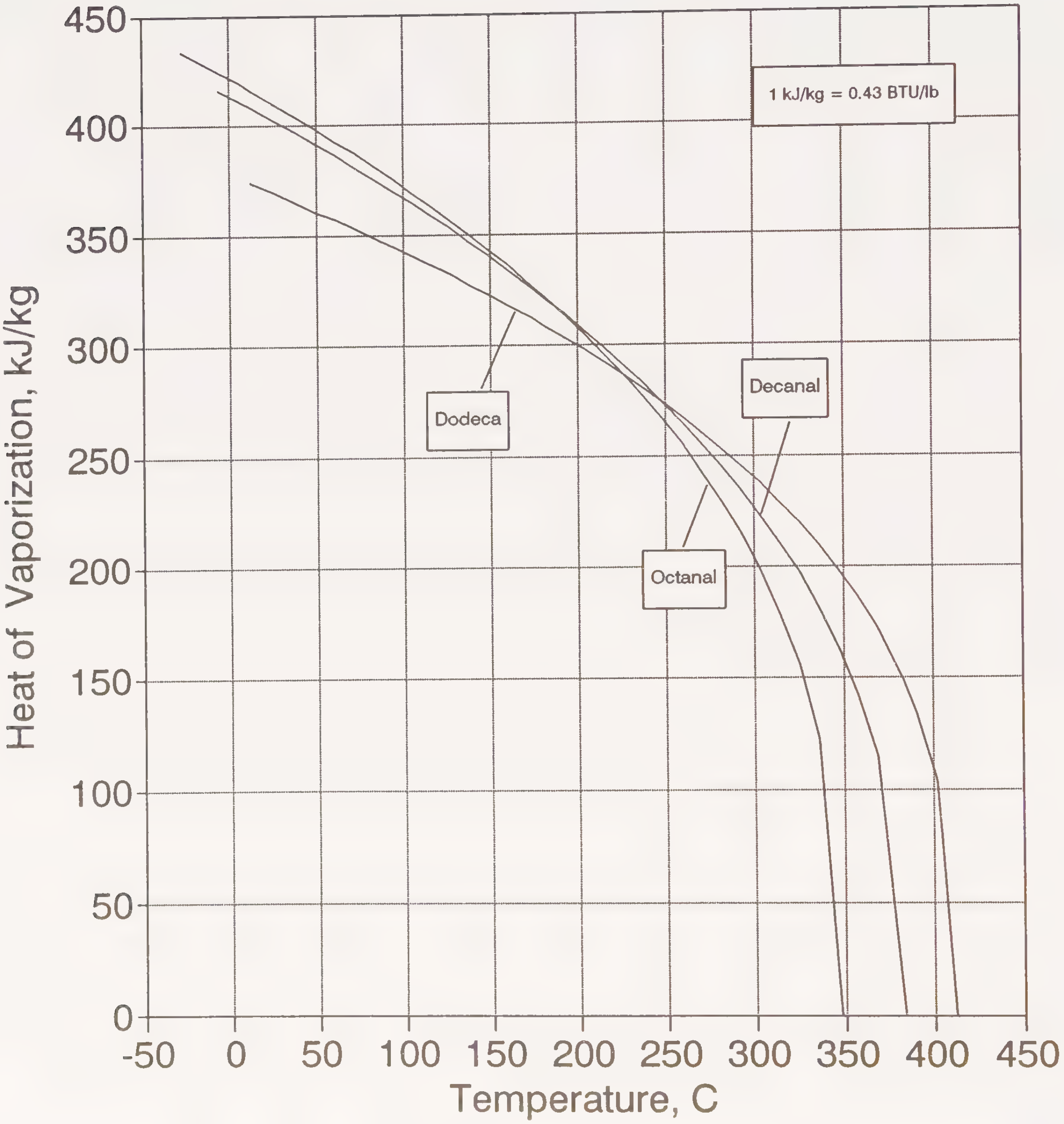

Figure 2-2 Heat of Vaporization

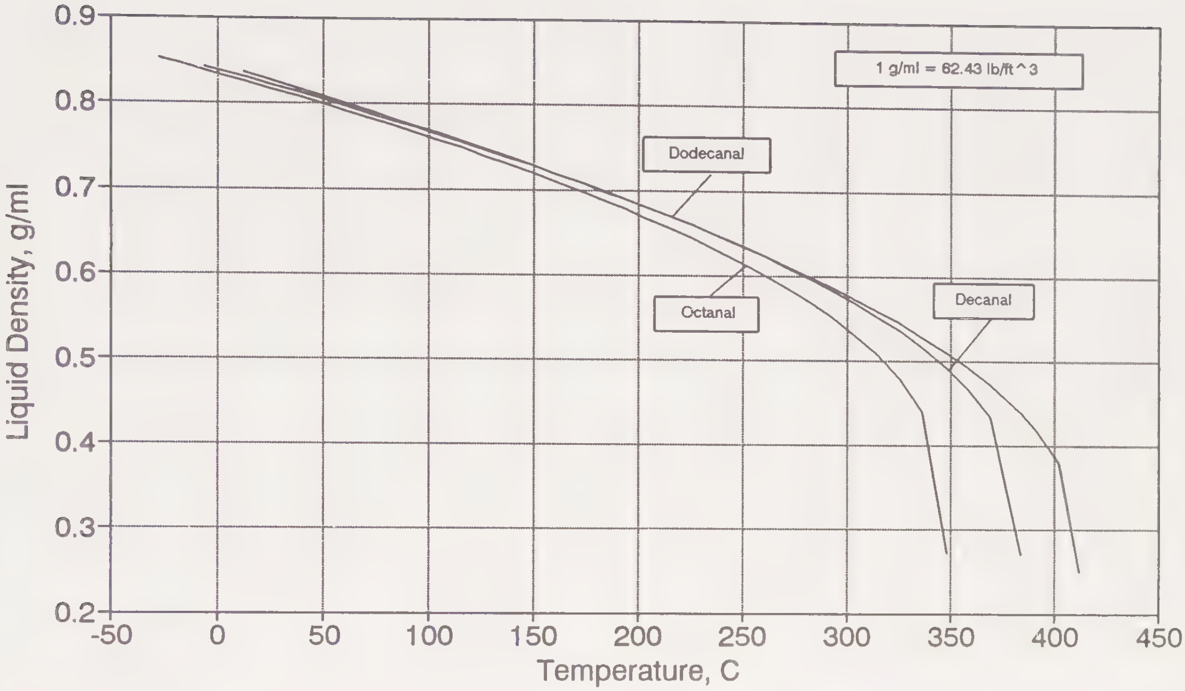

Figure 2-3 Liquid Density

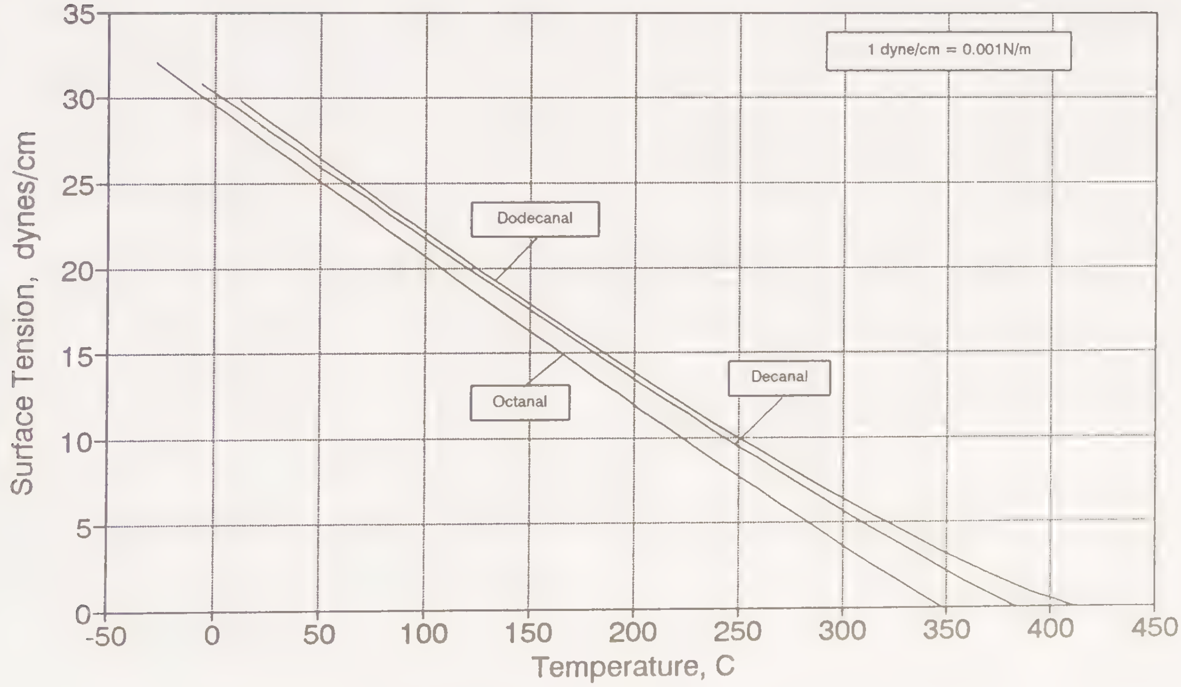

Figure 2-4 Surface Tension

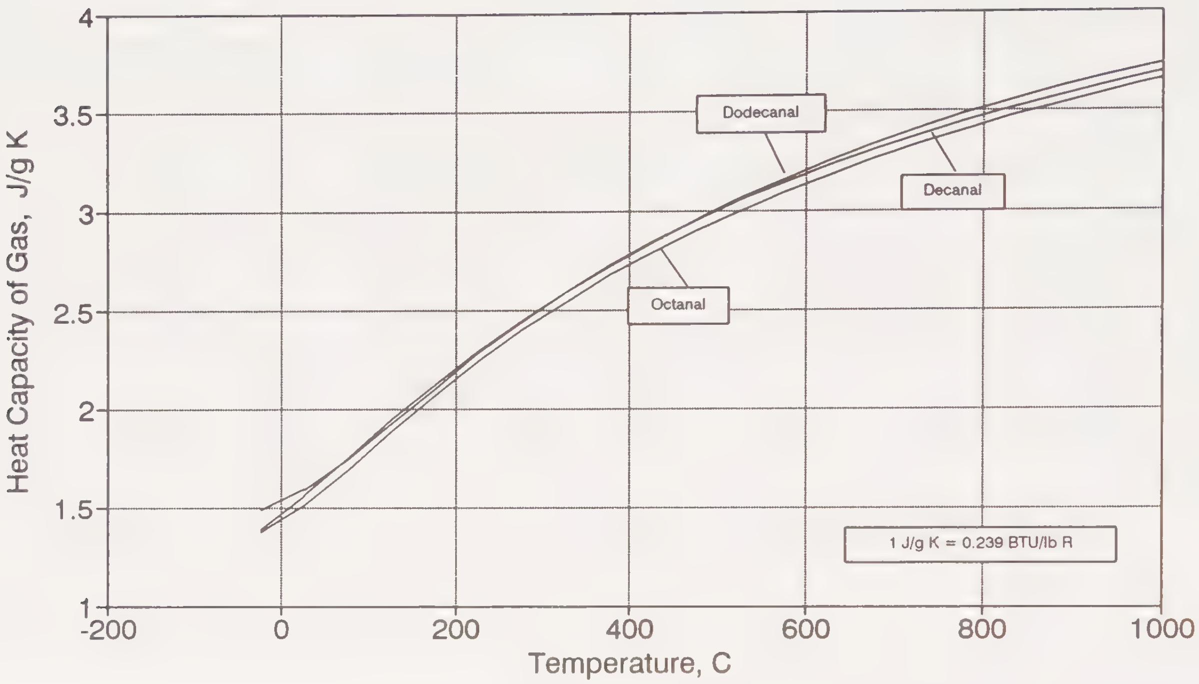

Figure 2-5 Heat Capacity of Gas

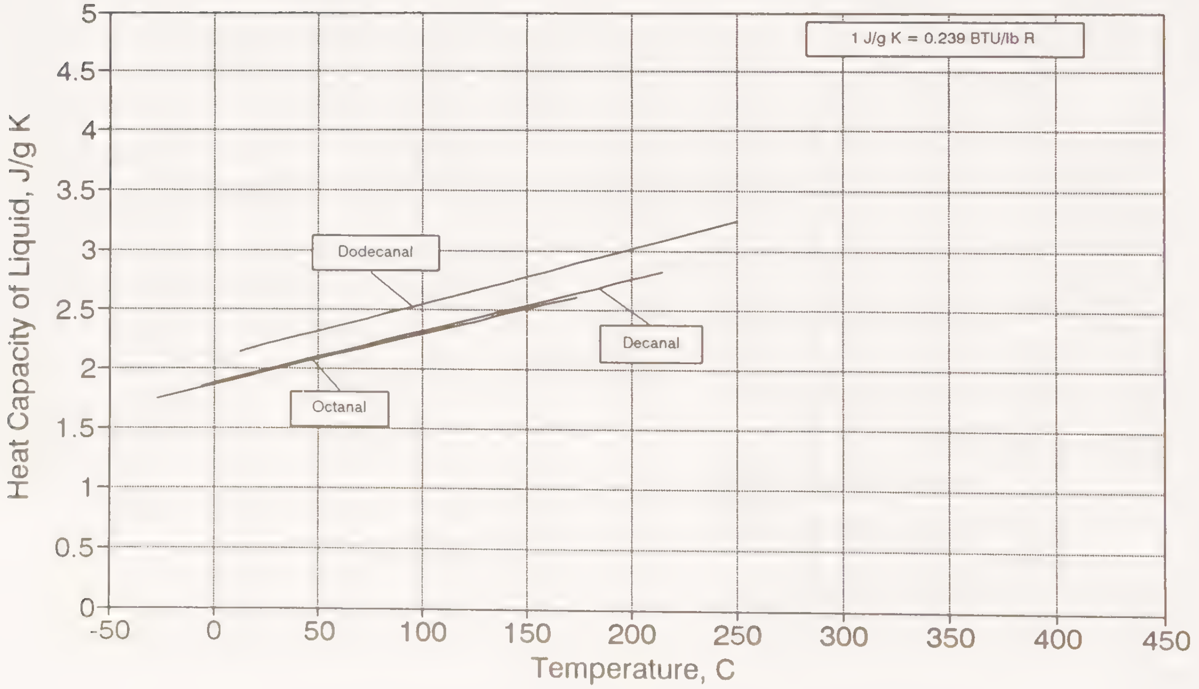

Figure 2-6 Heat Capacity of Liquid

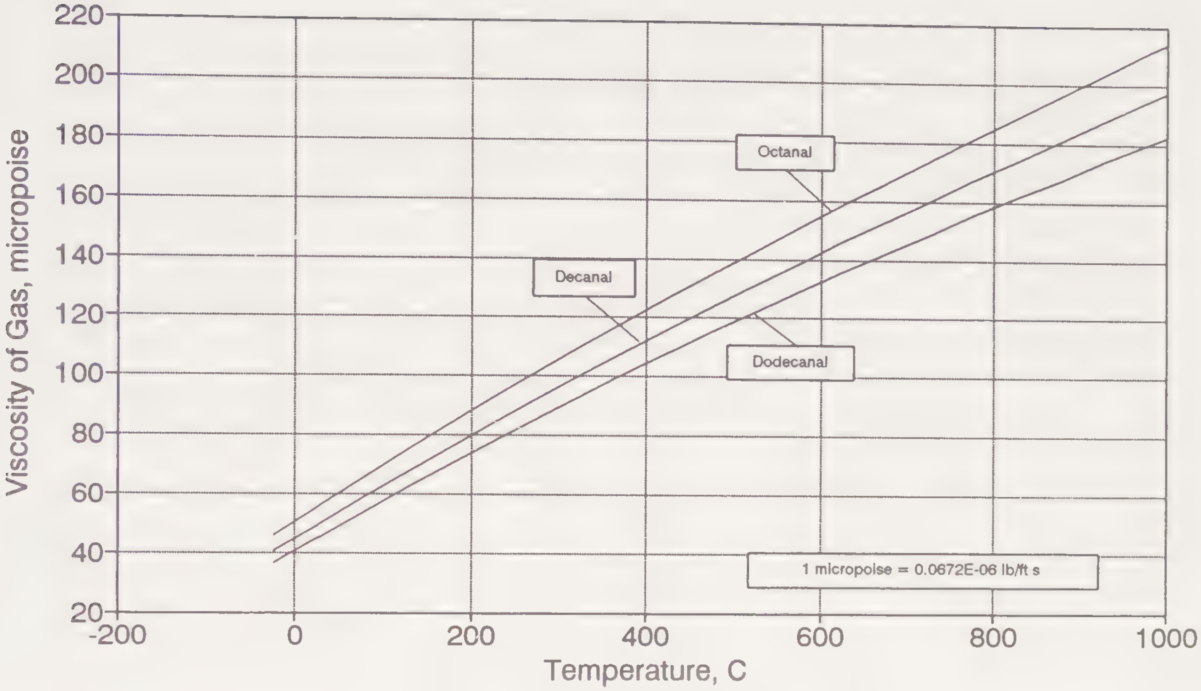

Figure 2-7 Viscosity of Gas

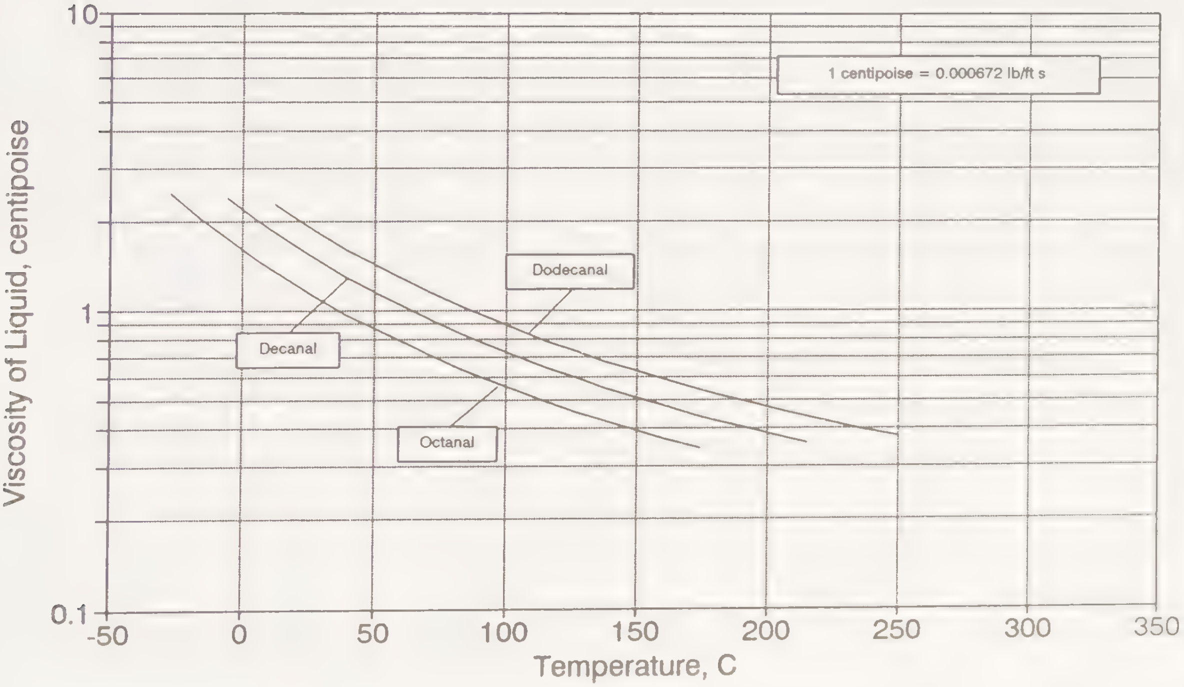

Figure 2-8 Viscosity of Liquid

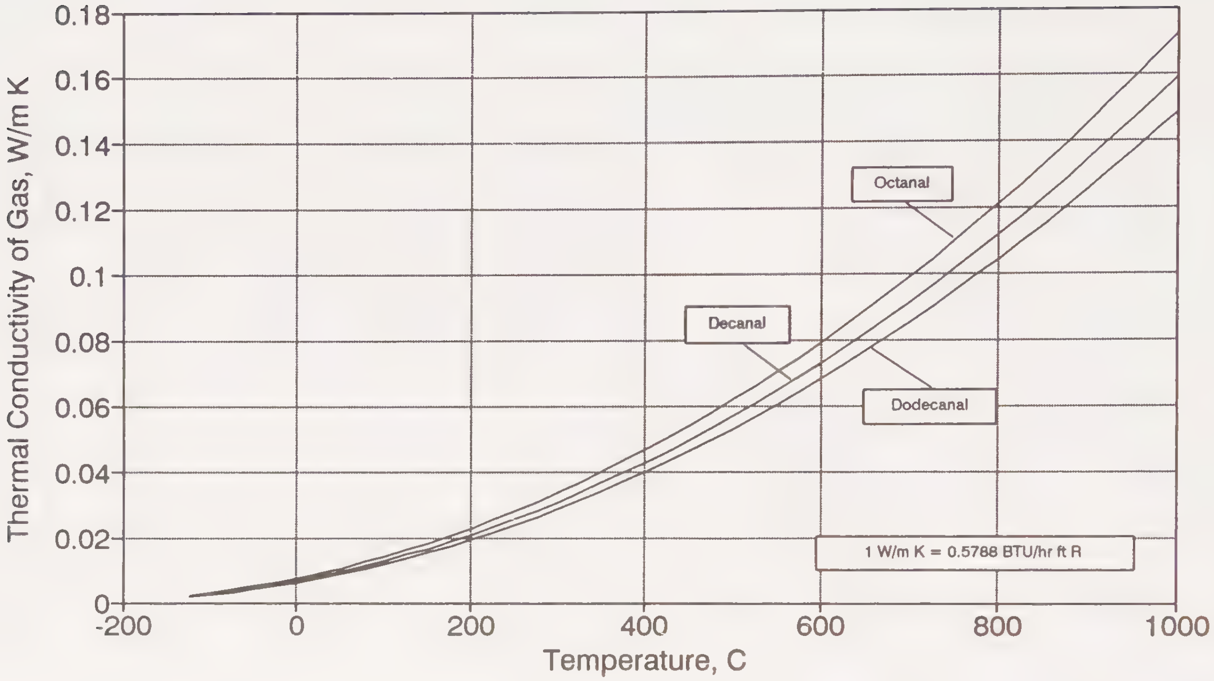

Figure 2-9 Thermal Conductivity of Gas

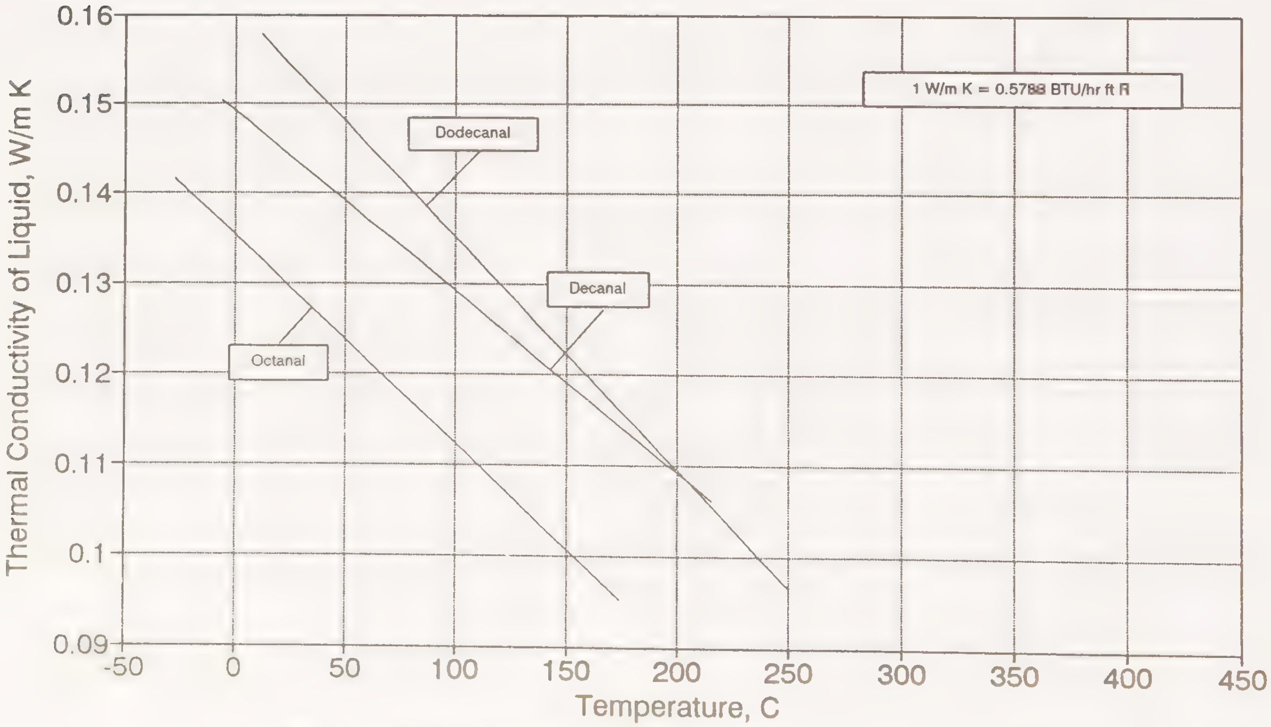

Figure 2-10 Thermal Conductivity of Liquid

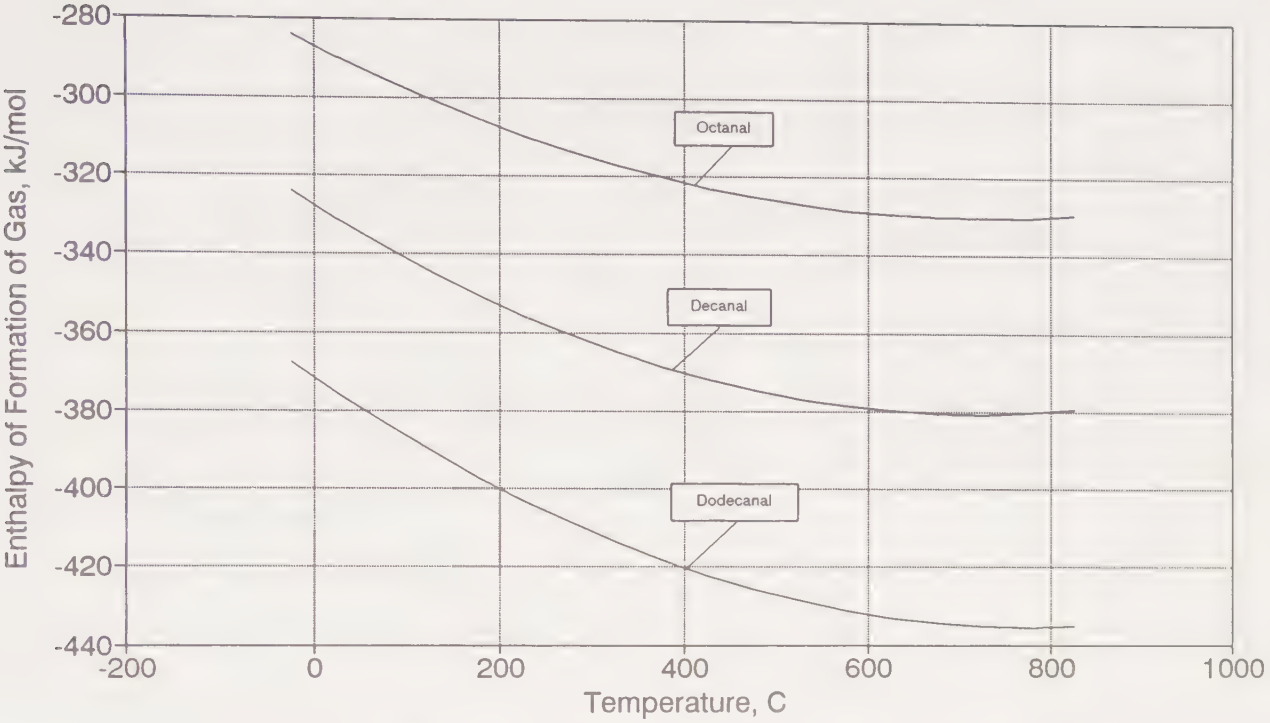

Figure 2-11 Enthalpy of Formation of Gas

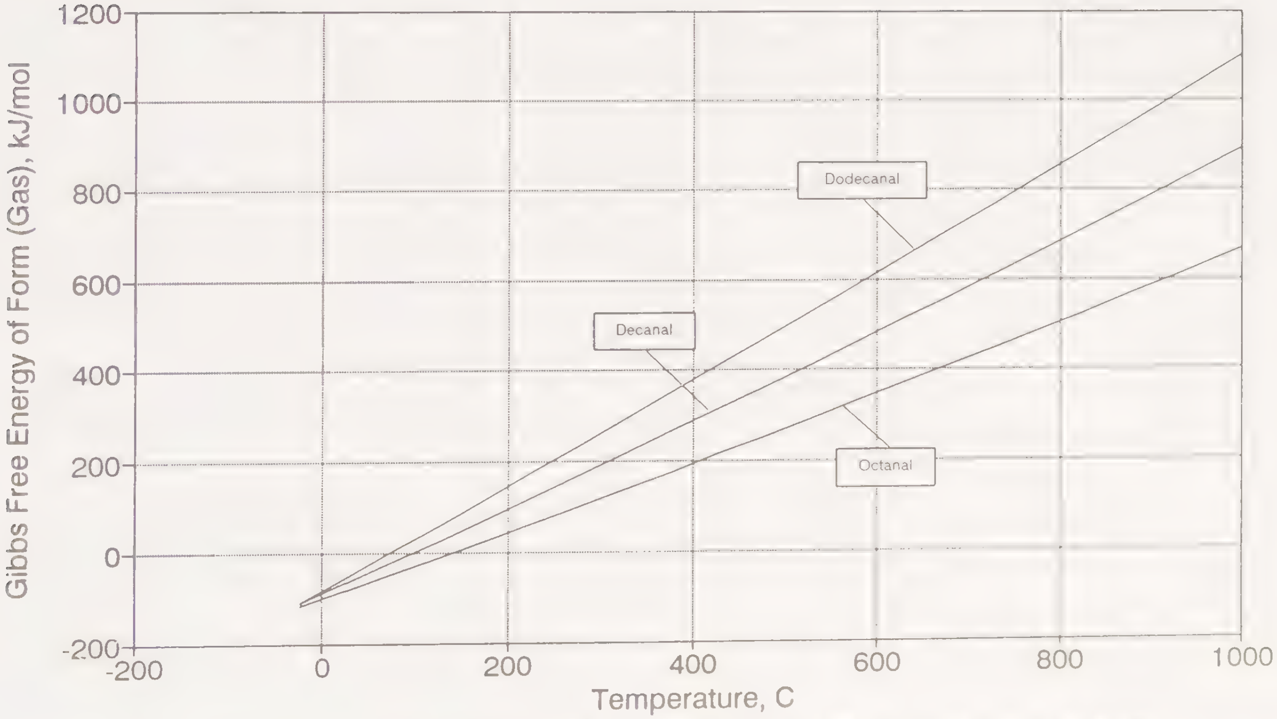

Figure 2-12 Gibbs Free Energy of Formation of Gas

Chapter 3

C_5 TO C_7 NORMAL ACIDS

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 3-1

Property data from the literature (2,3,8,21-23,33-36,63-65,75,77-88) are given in Table 3-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 3-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 3-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 5%.

LIQUID DENSITY - Figure 3-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

SURFACE TENSION - Figure 3-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 3-5 and 3-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 5% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in rough agreement with data. Errors are about 25% or less in most cases.

VISCOSITY - Figures 3-7 and 3-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 3% or less in most cases.

THERMAL CONDUCTIVITY - Figures 3-9 and 3-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is favorable with possible errors of 5% in most cases.

ENTHALPY OF FORMATION - Figure 3-11

The data compilation of DIPPR project(5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 3-12

The data compilation of DIPPR project(5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 3-1 Physical Properties

1. Name	Pentanoic Acid	Hexanoic Acid	Heptanoic Acid
2. Formula	C5H10O2	C6H12O2	C7H14O2
3. Molecular Weight, g/mol	102.133	116.160	130.187
4. Critical Temperature, K	651.00	667.00	680.00
5. Critical Pressure, bar	38.100	33.500	29.900
6. Critical Volume, ml/mol	336.00	389.00	442.00
7. Critical Compressibility Factor	0.237	0.235	0.234
8. Acentric Factor	0.6269	0.6701	0.7173
9. Melting Point, K	239.15	270.15	265.83
10. Boiling Point @ 1 atm, K	458.65	478.85	496.15
11. Heat of Vaporization @ BP, kJ/kg	475.26	448.70	397.36
12. Density of Liquid @ 25 C, g/ml	0.934	0.921	0.913
13. Surface Tension @ 25 C, dynes/cm	26.81	26.78	27.75
14. Heat Capacity of Gas @ 25 C, J/g K	1.353	1.387	1.414
15. Heat Capacity of Liquid @ 25 C, J/g K	2.059	2.262	2.038
16. Viscosity of Gas @ 25 C, micropoise	65.10	60.79	57.42
17. Viscosity of Liquid @ 25 C, centipoise	2.012	2.843	3.847
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.011	0.011	0.010
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.142	0.144	0.142
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-491.00	-514.38	-535.53
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-347.13	-341.37	-333.60
22. Flash Point, K	369.15	374.82	383.00
23. Autoignition Temperture, K	673.15	653.15	650.00
24. Lower Explosion Limit in Air, vol %	1.6	1.3	1.1
25. Upper Explosion Limit in Air, vol %	9.6	8.2	7.2
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

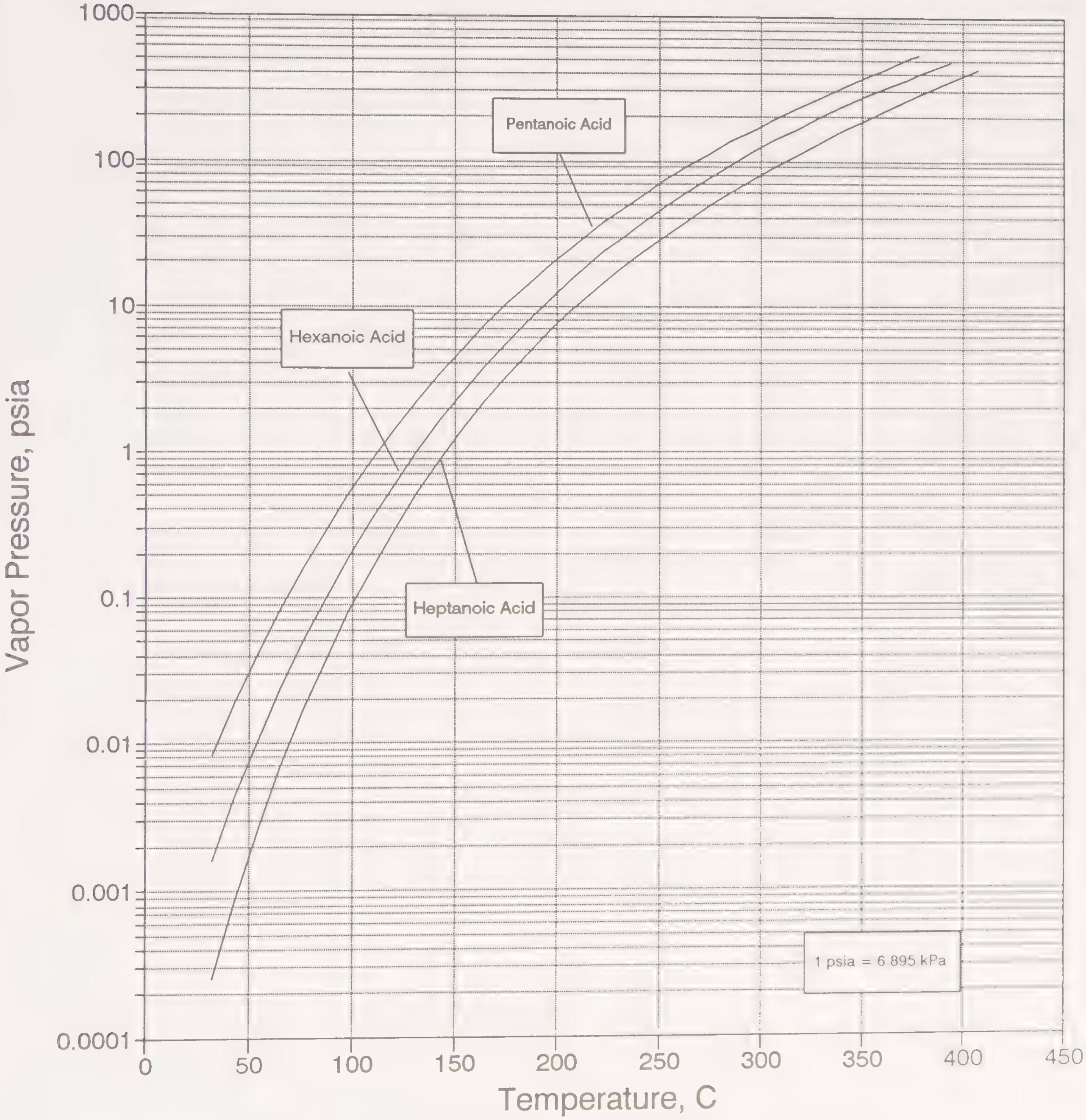

Figure 3-1 Vapor Pressure

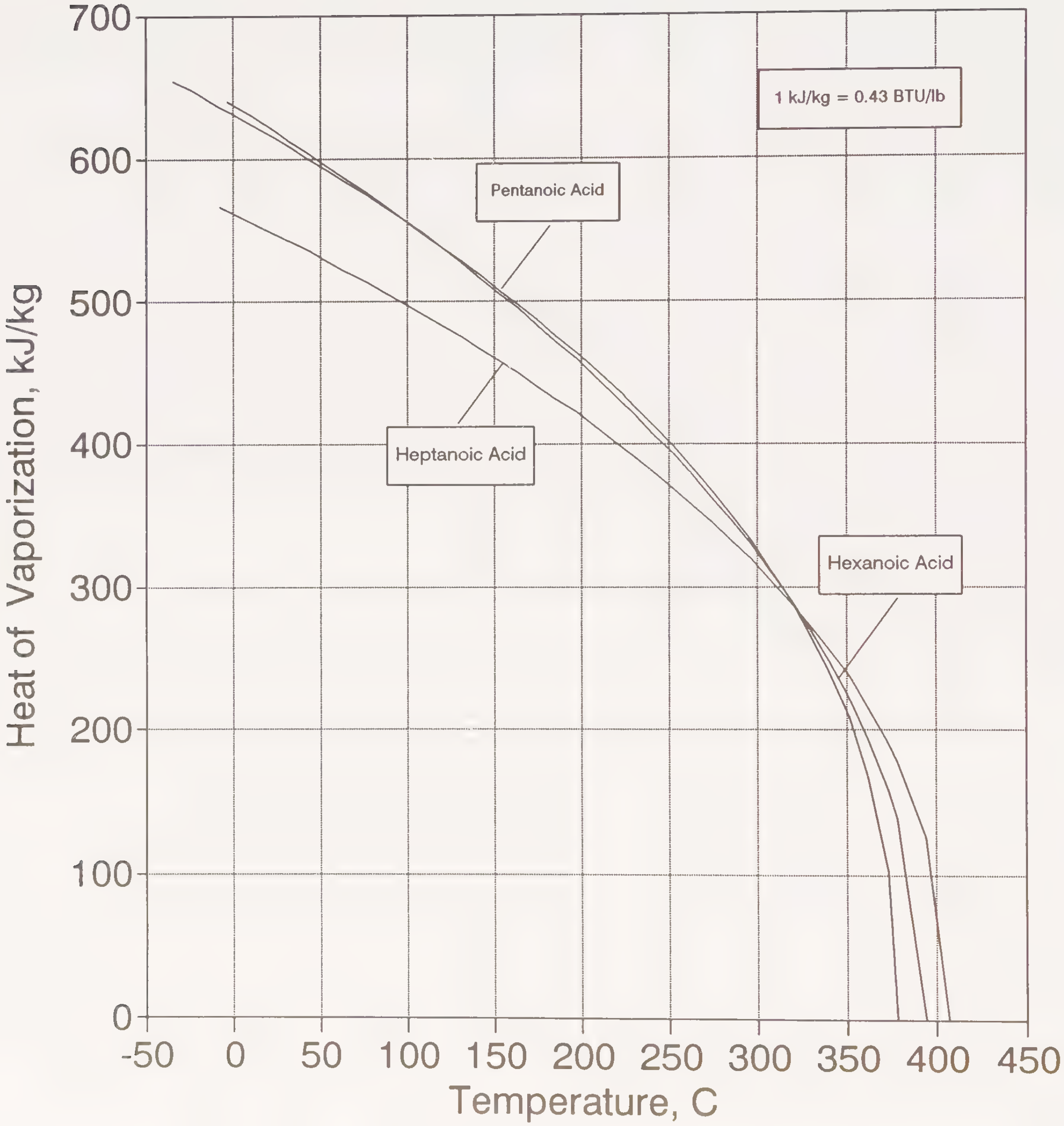

Figure 3-2 Heat of Vaporization

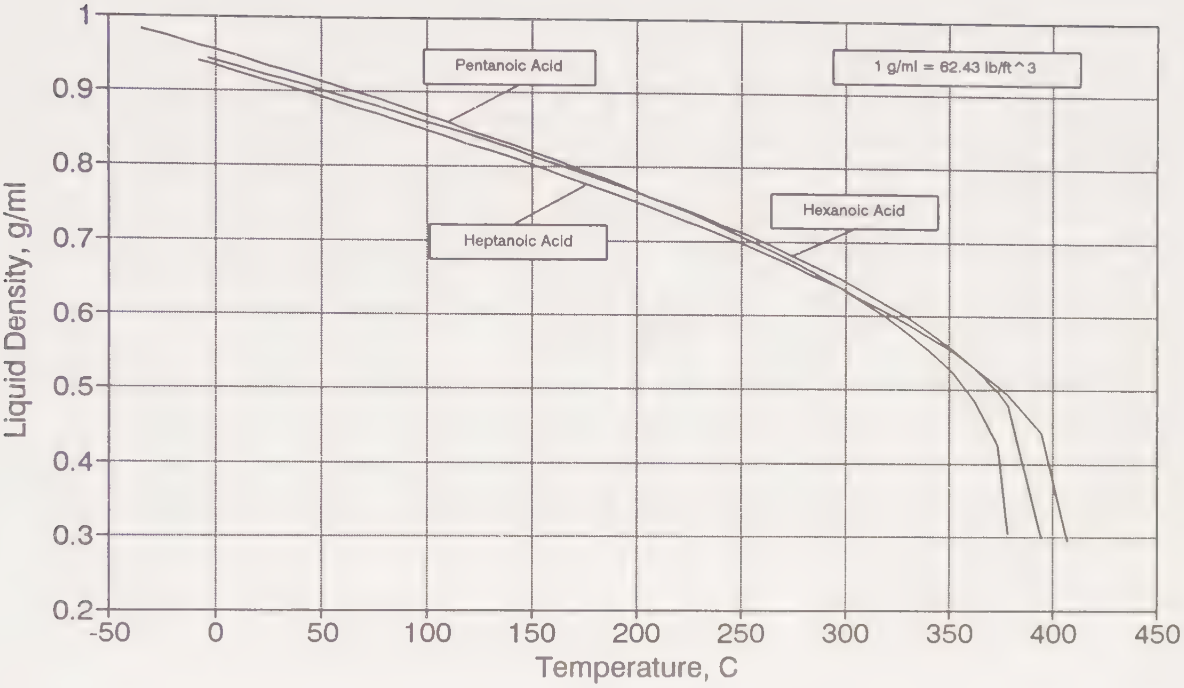

Figure 3-3 Liquid Density

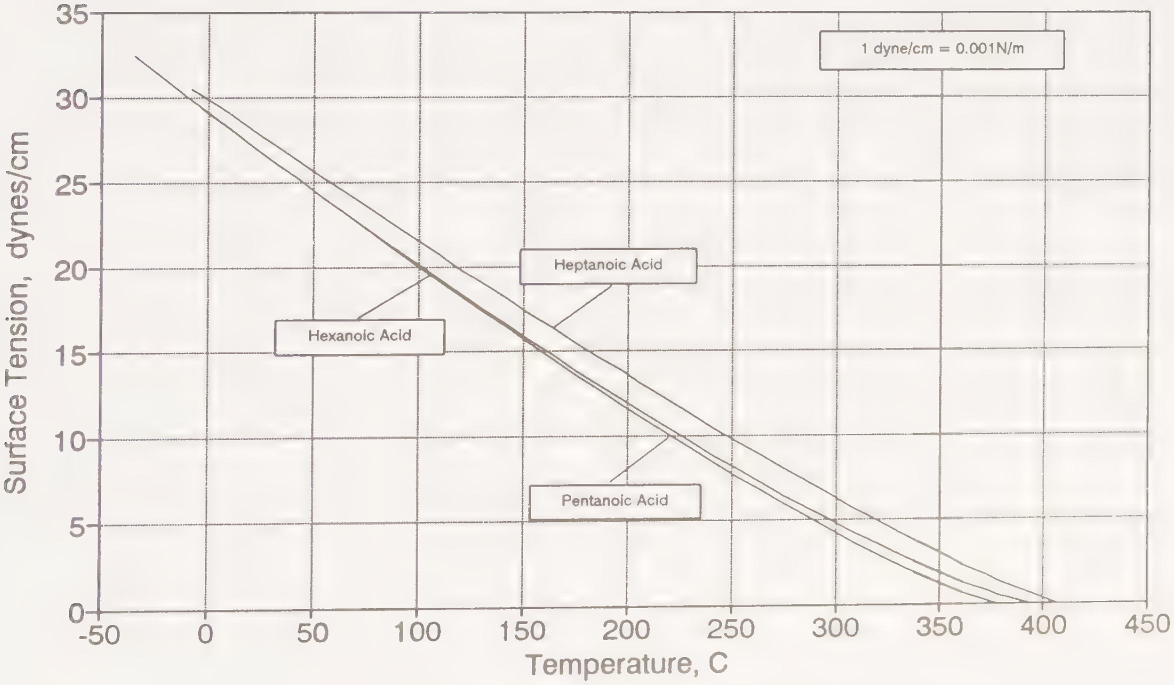

Figure 3-4 Surface Tension

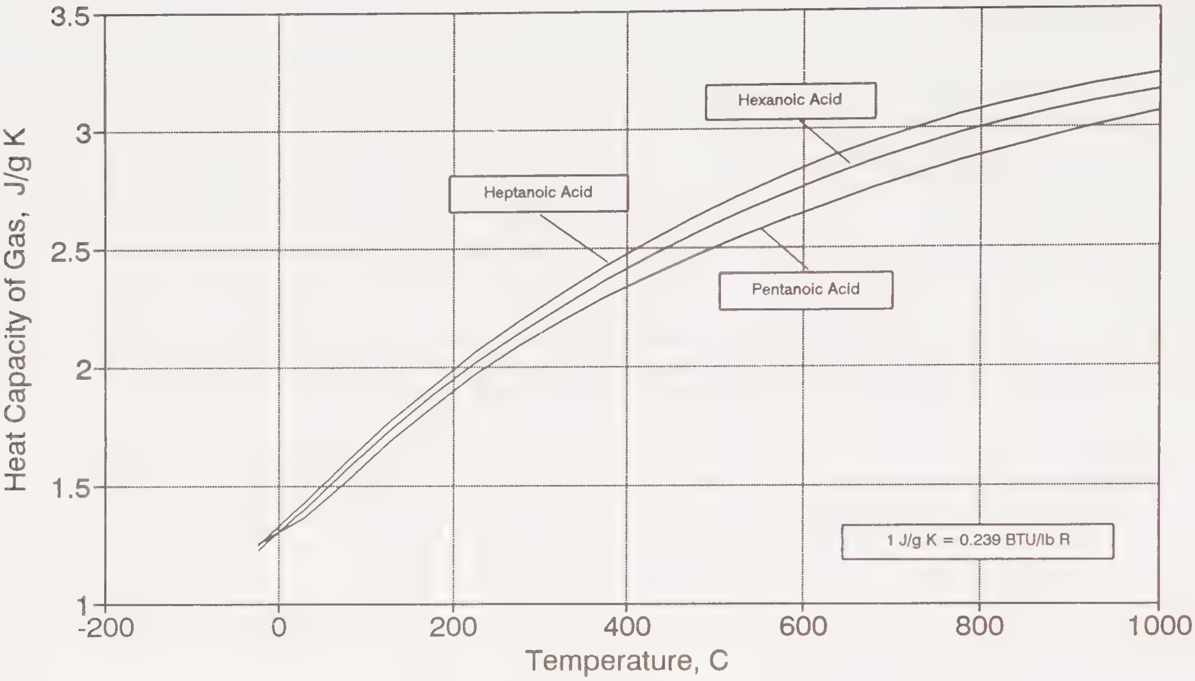

Figure 3-5 Heat Capacity of Gas

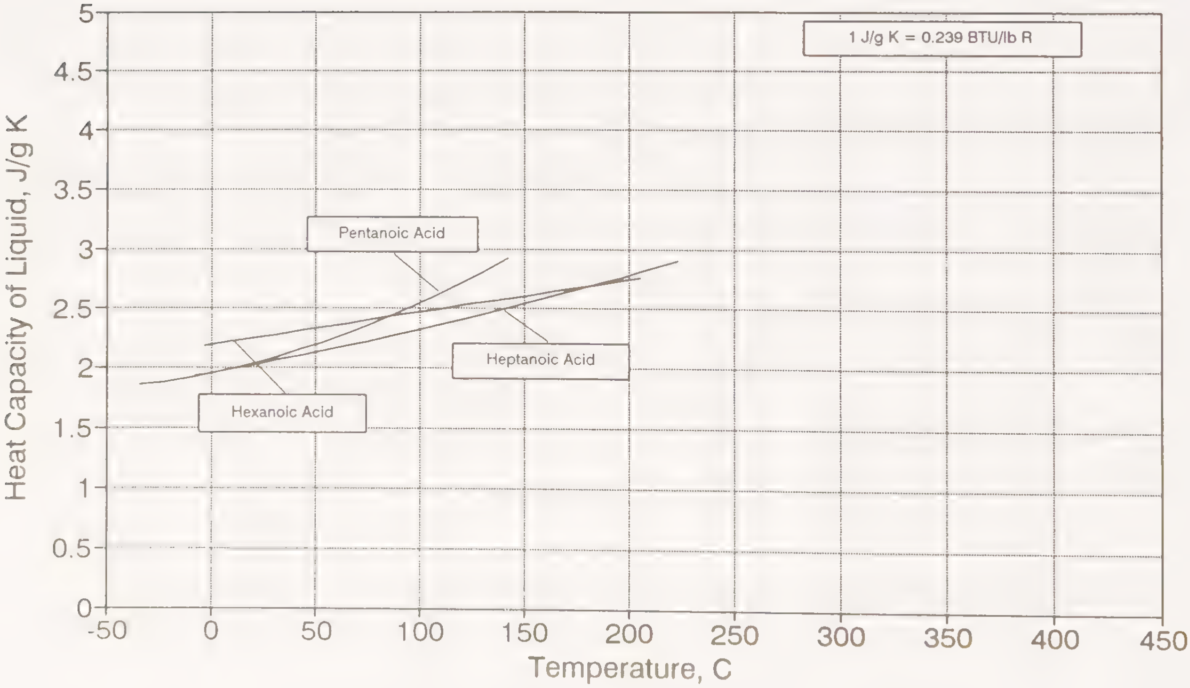

Figure 3-6 Heat Capacity of Liquid

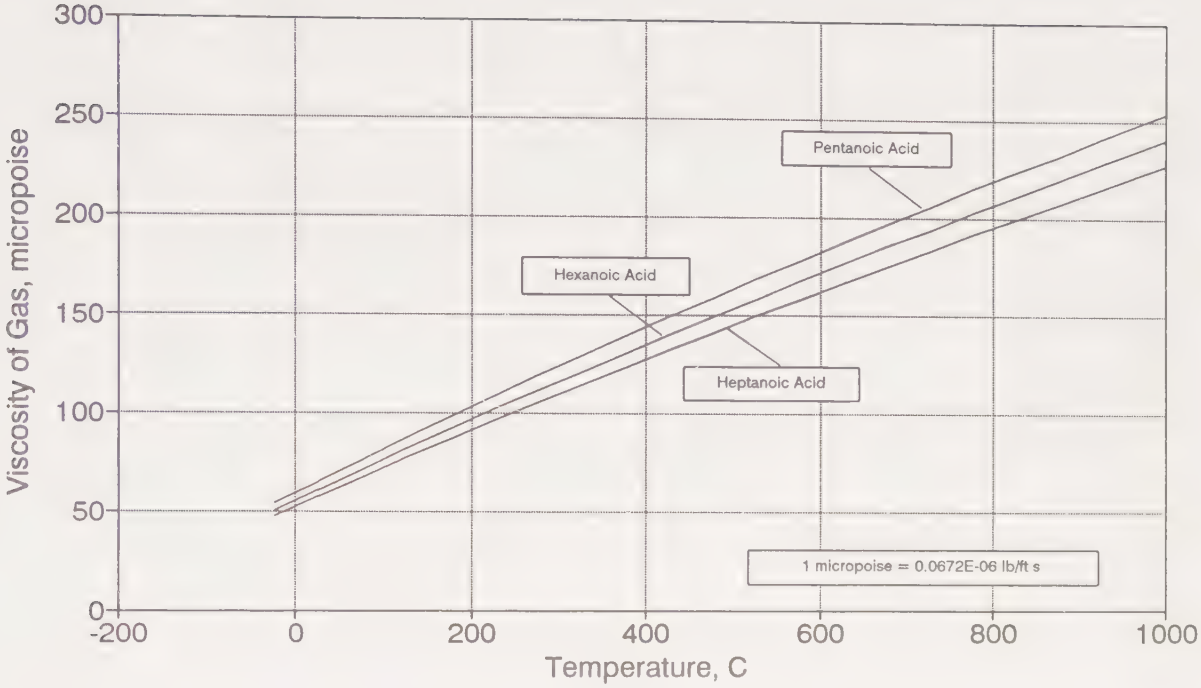

Figure 3-7 Viscosity of Gas

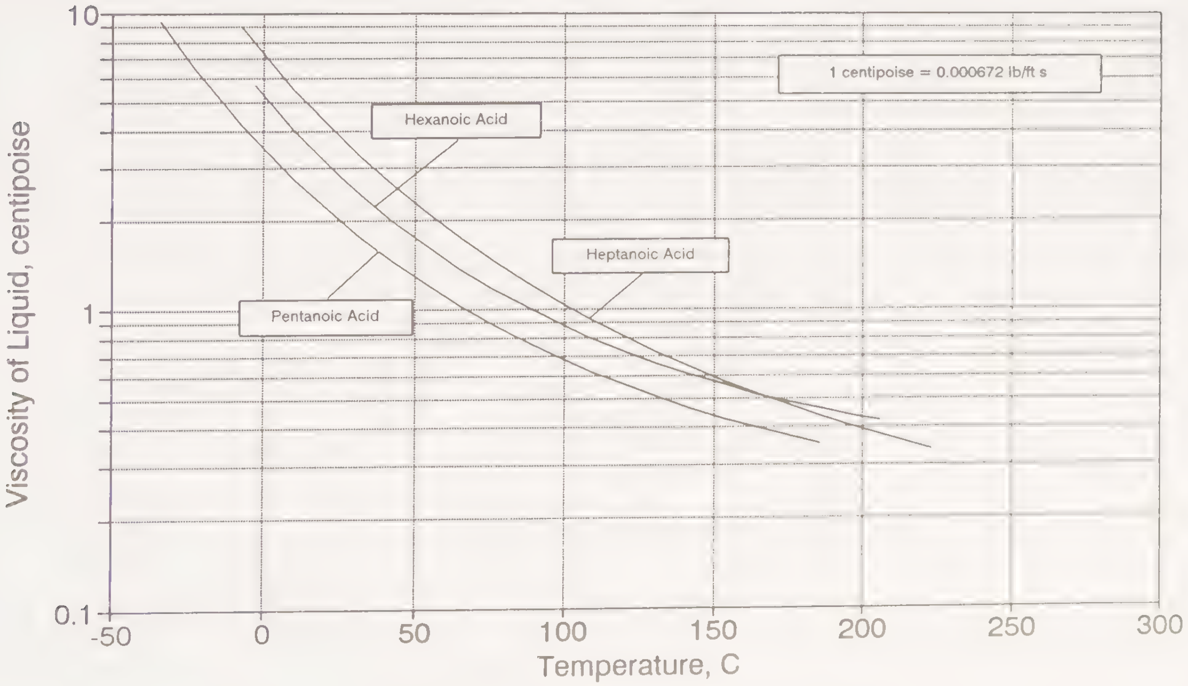

Figure 3-8 Viscosity of Liquid

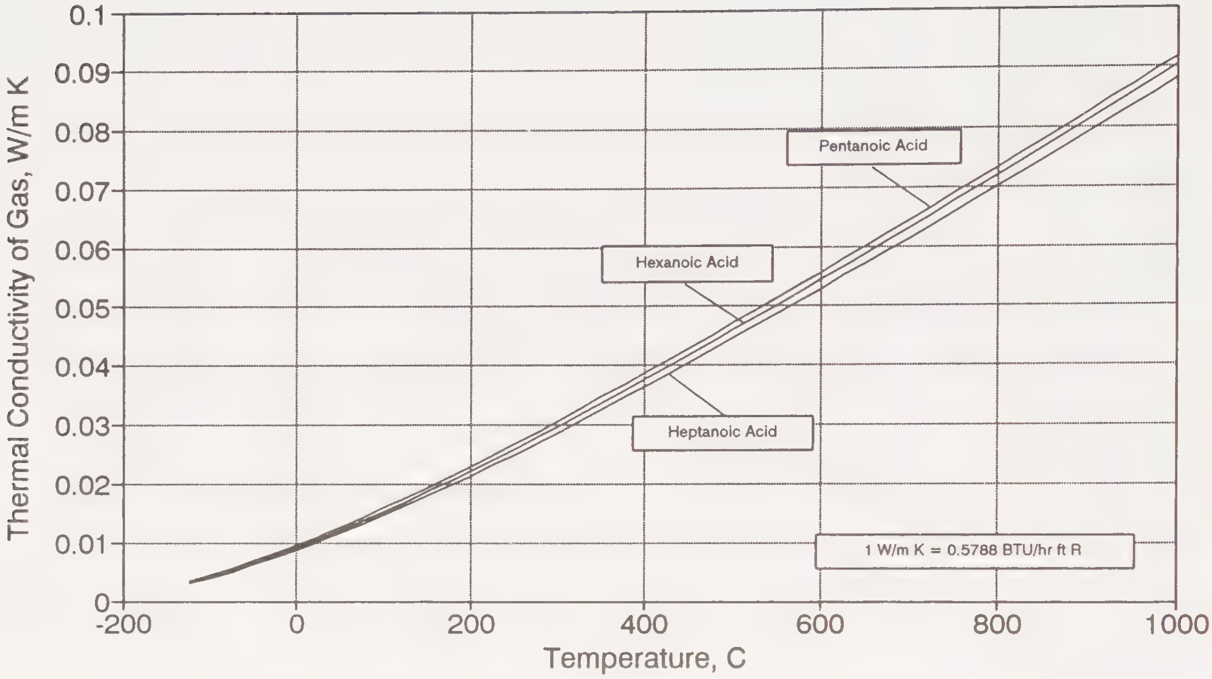

Figure 3-9 Thermal Conductivity of Gas

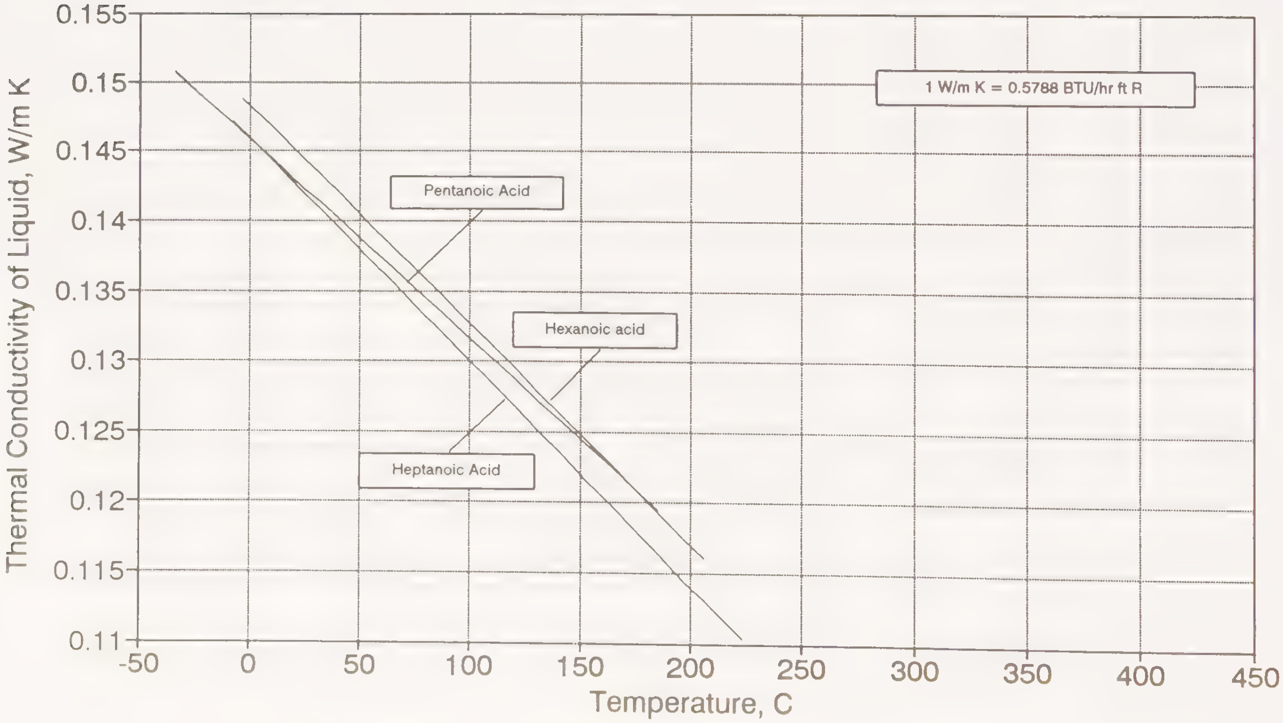

Figure 3-10 Thermal Conductivity of Liquid

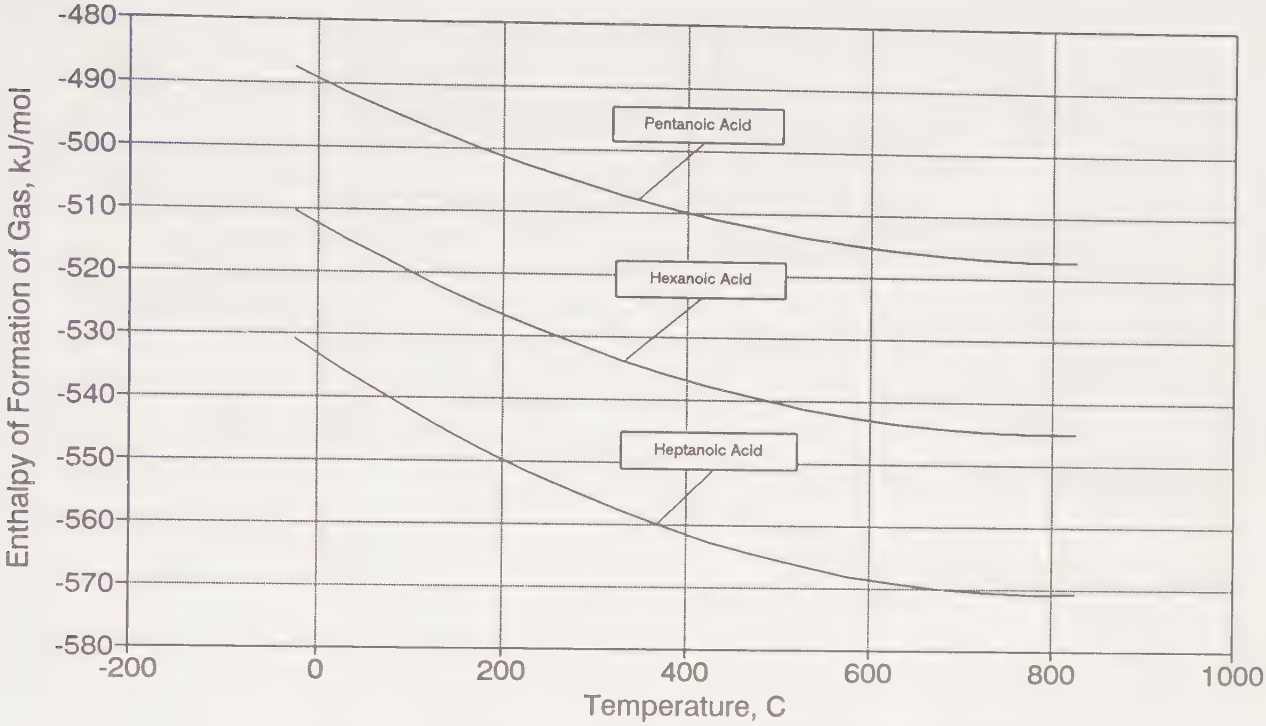

Figure 3-11 Enthalpy of Formation of Gas

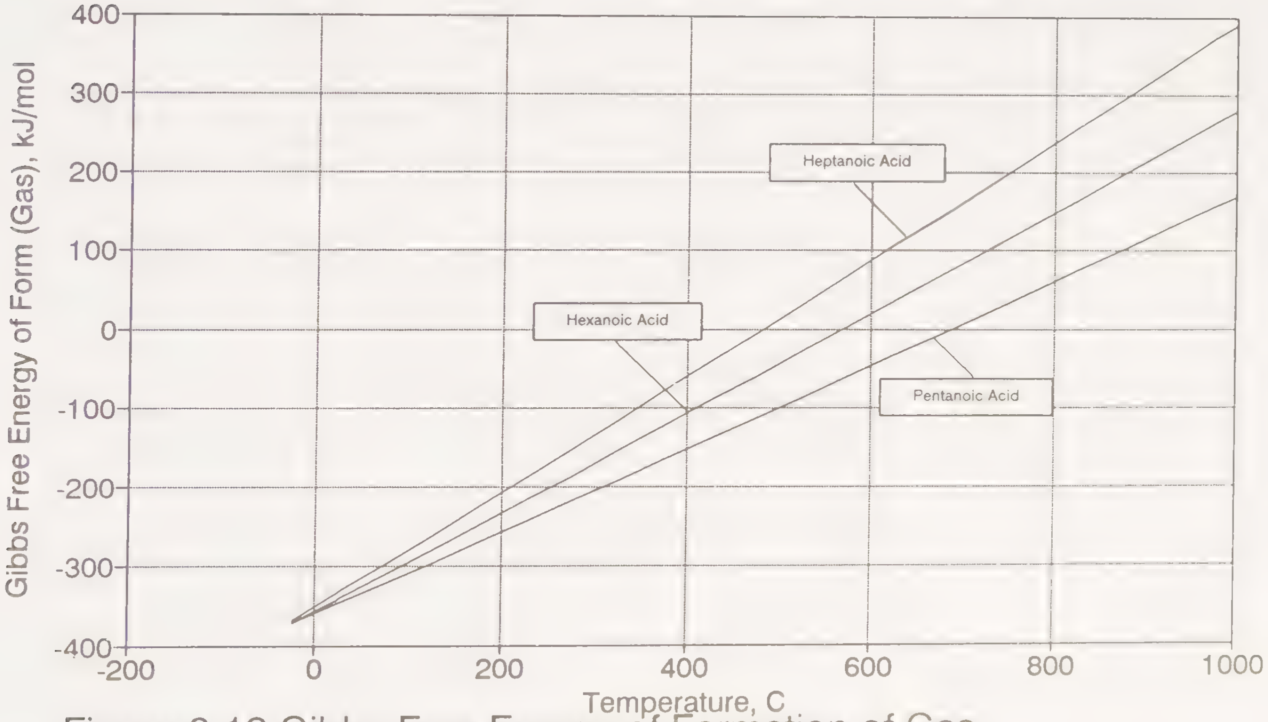

Figure 3-12 Gibbs Free Energy of Formation of Gas

Chapter 4

C_8, C_{10} AND C_{12} NORMAL ACIDS

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 4-1

Property data from the literature (2,3,8,21,63-65,73-80,85-87,89-92) are given in Table 4-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 4-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 4-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 5%.

LIQUID DENSITY - Figure 4-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

SURFACE TENSION - Figure 4-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 4-5 and 4-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 5% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in rough agreement with data. Errors are about 5% or less in most cases except octanoic acid(possible 25% error).

VISCOSITY - Figures 4-7 and 4-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 10% or less in most cases.

THERMAL CONDUCTIVITY - Figures 4-9 and 4-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 4-11

The data compilation of DIPPR project(5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 4-12

The data compilation of DIPPR project(5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 4-1 Physical Properties

1. Name	Octanoic Acid	Decanoic Acid	Dodecanoic Acid
2. Formula	C8H16O2	C10H20O2	C12H24O2
3. Molecular Weight, g/mol	144.214	172.268	200.321
4. Critical Temperature, K	692.00	713.00	734.00
5. Critical Pressure, bar	26.900	22.500	19.400
6. Critical Volume, ml/mol	494.00	600.00	705.00
7. Critical Compressibility Factor	0.231	0.228	0.224
8. Acentric Factor	0.7792	0.8774	0.9671
9. Melting Point, K	289.65	304.75	317.15
10. Boiling Point @ 1 atm, K	513.05	543.15	571.85
11. Heat of Vaporization @ BP, kJ/kg	390.46	356.75	310.45
12. Density of Liquid @ BP, g/ml	0.722	0.699	0.666
13. Surface Tension @ BP, dynes/cm	11.44	10.52	9.70
14. Heat Capacity of Gas @ 25 C, J/g K	1.432	1.465	1.490
15. Heat Capacity of Liquid @ BP, J/g K	2.862	3.390	------
16. Viscosity of Gas @ 25 C, micropoise	54.31	49.57	46.12
17. Viscosity of Liquid @ BP, centipoise	0.375	0.230	0.318
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.010	0.009	0.009
19. Thermal Conductivity of Liquid @ BP, W/m K	0.100	0.107	0.107
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-556.96	-595.60	-643.40
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-326.82	-307.26	-299.70
22. Flash Point, K	393.00	415.00	430.00
23. Autoignition Temperture, K	650.00	650.00	650.00
24. Lower Explosion Limit in Air, vol %	1.0	0.8	0.6
25. Upper Explosion Limit in Air, vol %	6.4	5.5	8.4
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

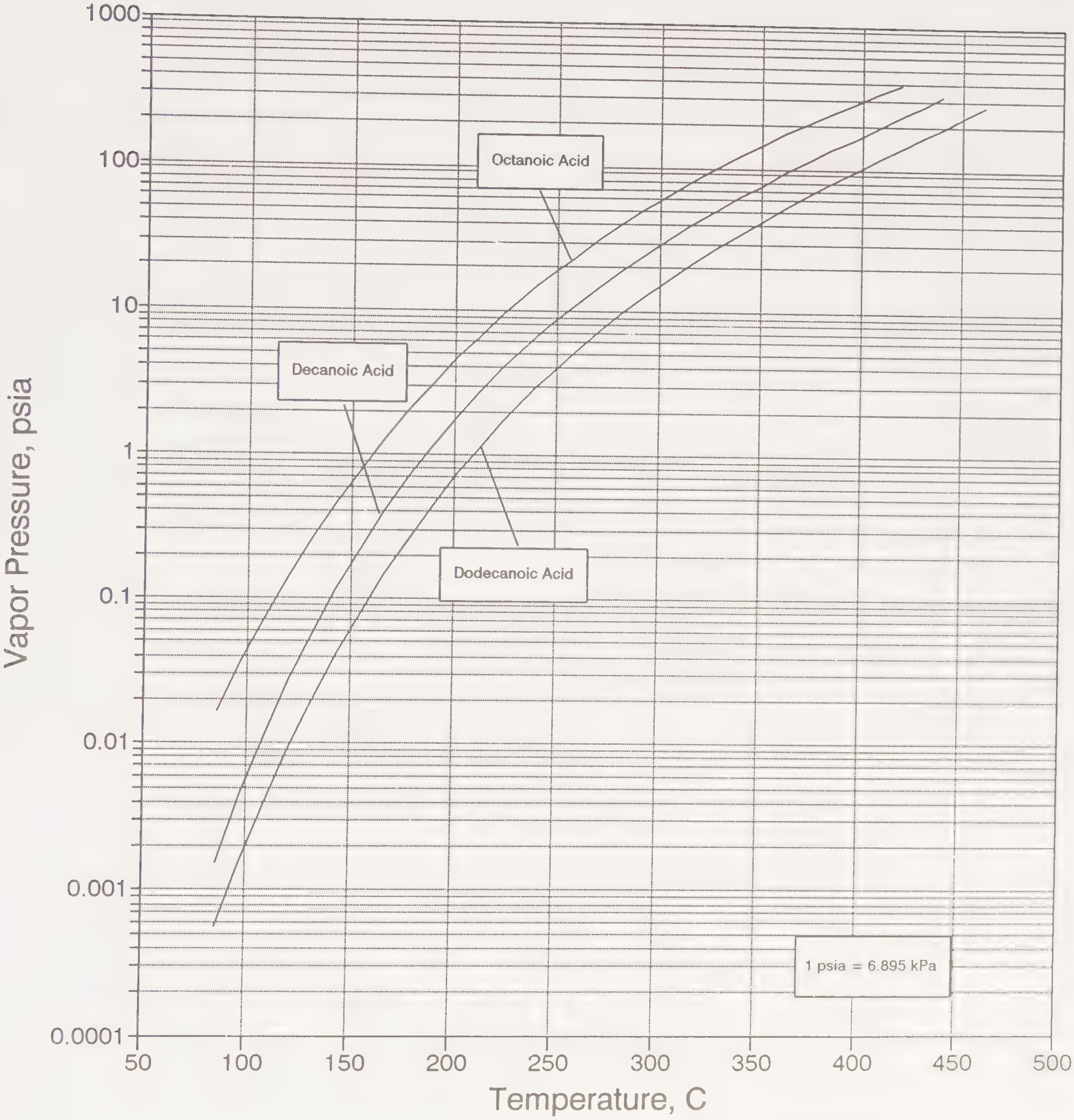

Figure 4-1 Vapor Pressure

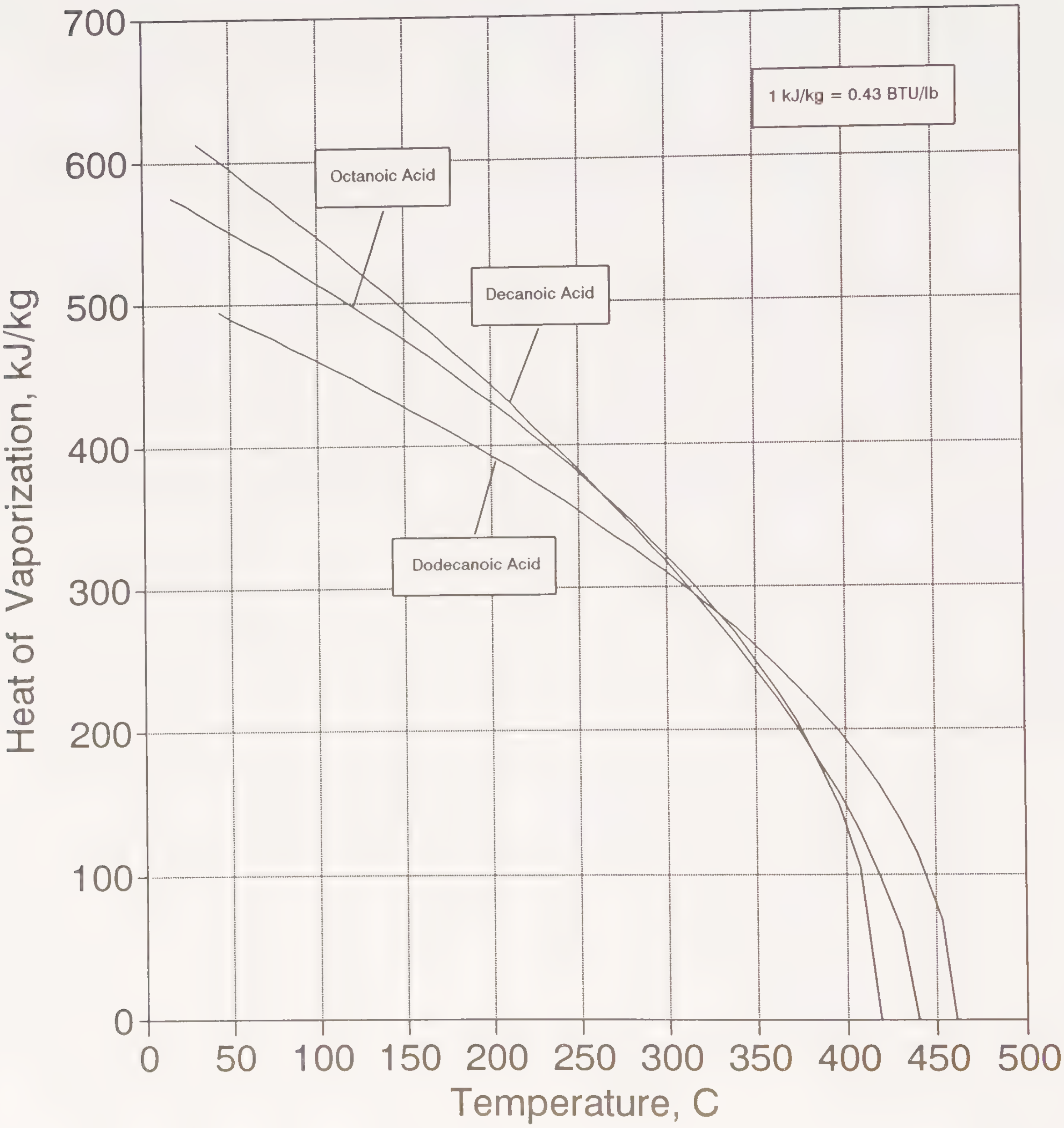

Figure 4-2 Heat of Vaporization

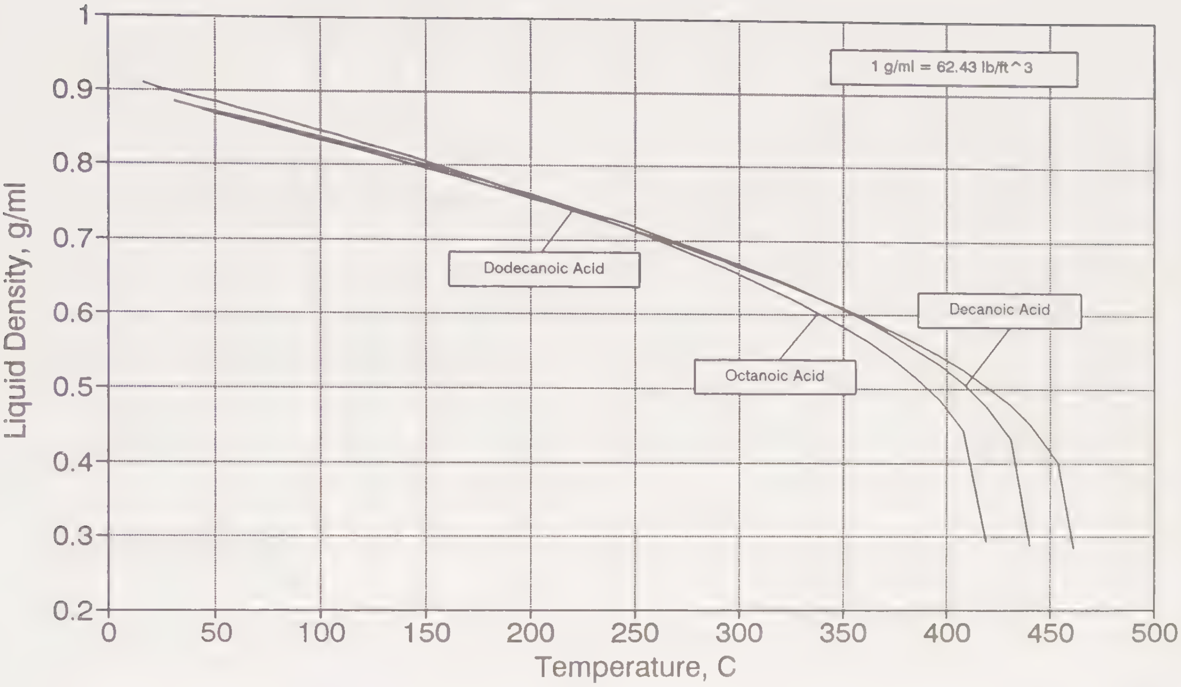

Figure 4-3 Liquid Density

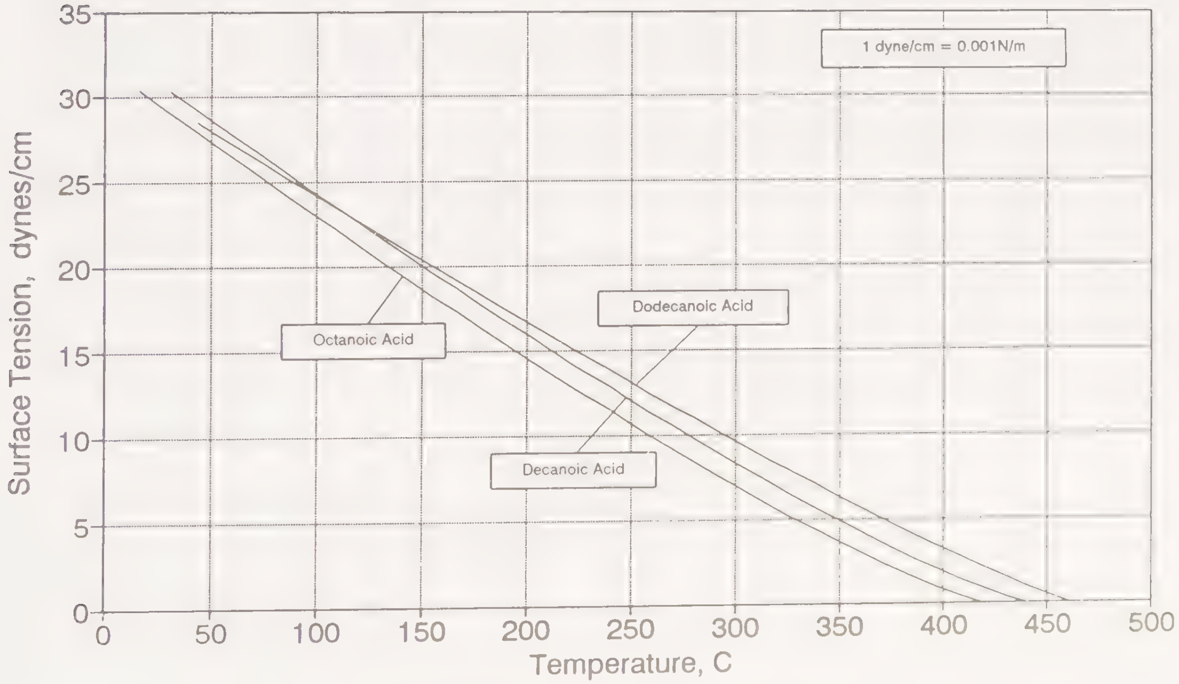

Figure 4-4 Surface Tension

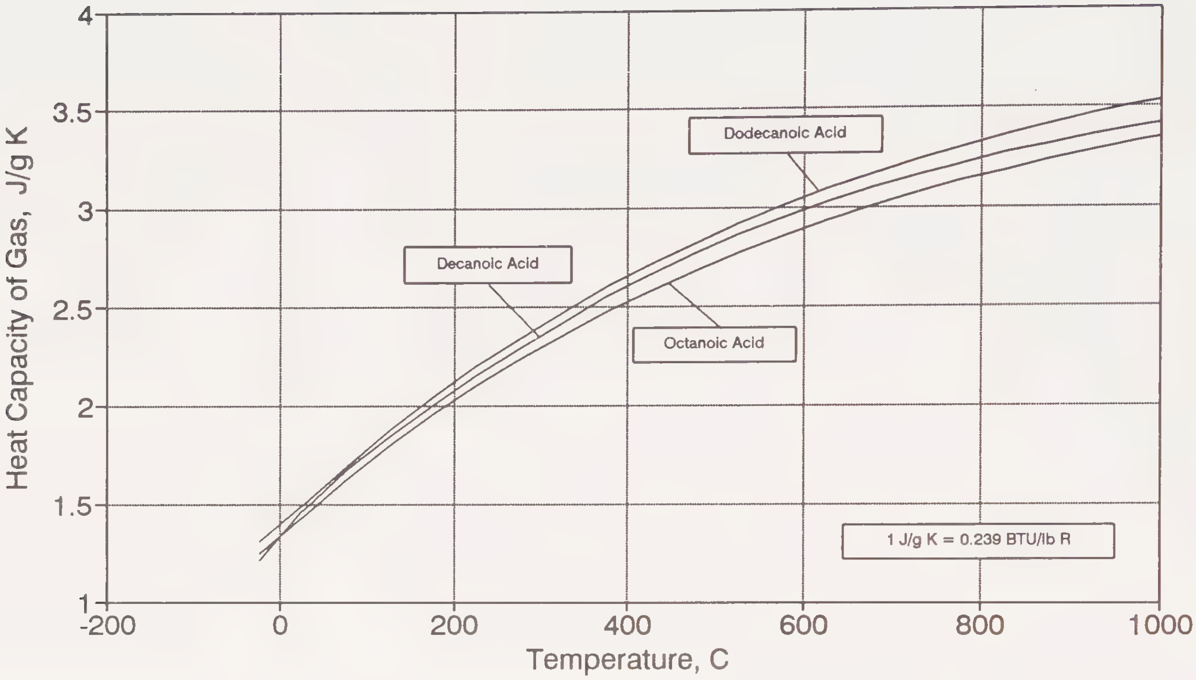

Figure 4-5 Heat Capacity of Gas

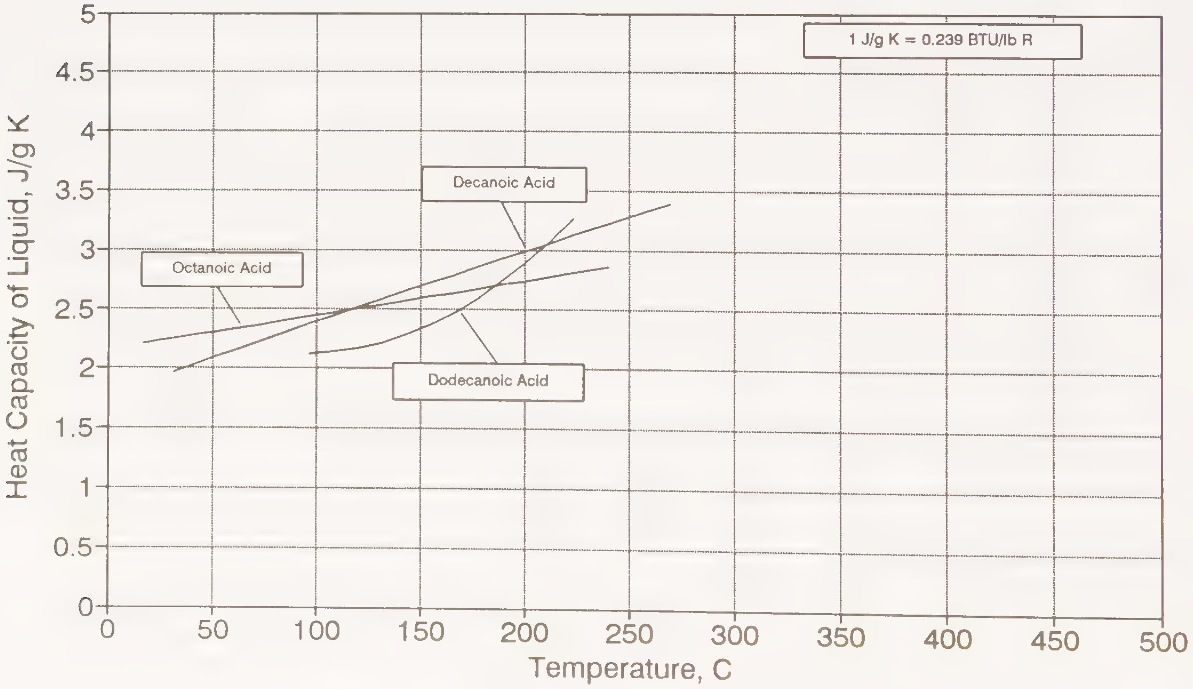

Figure 4-6 Heat Capacity of Liquid

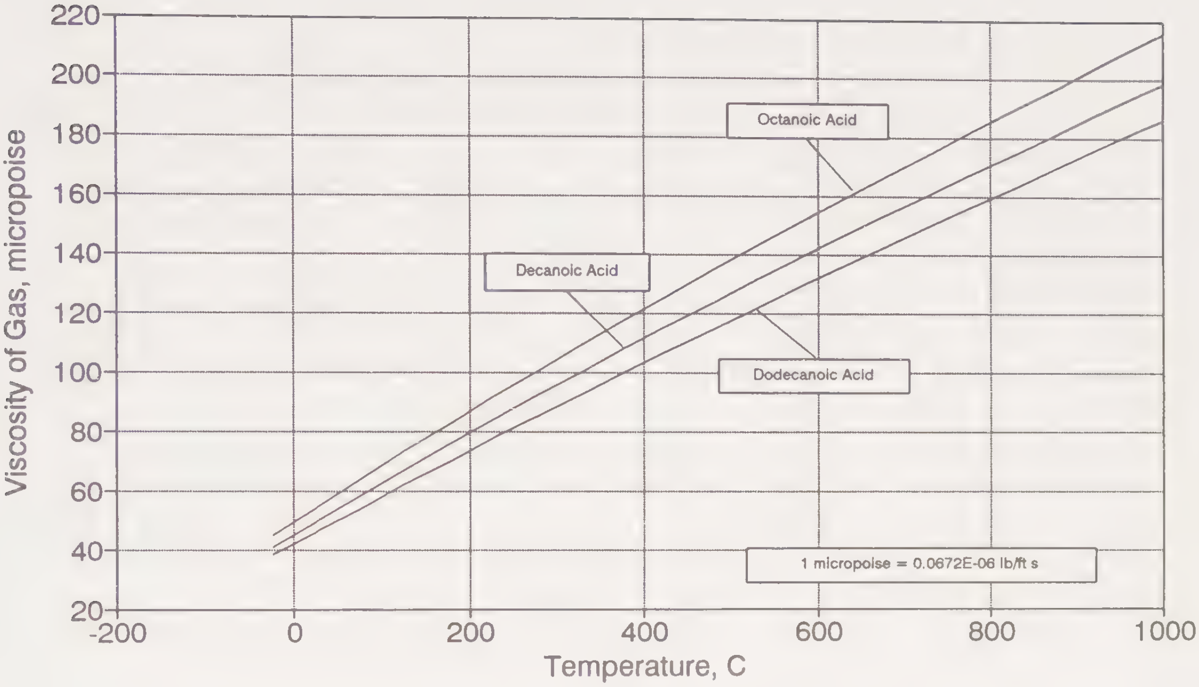

Figure 4-7 Viscosity of Gas

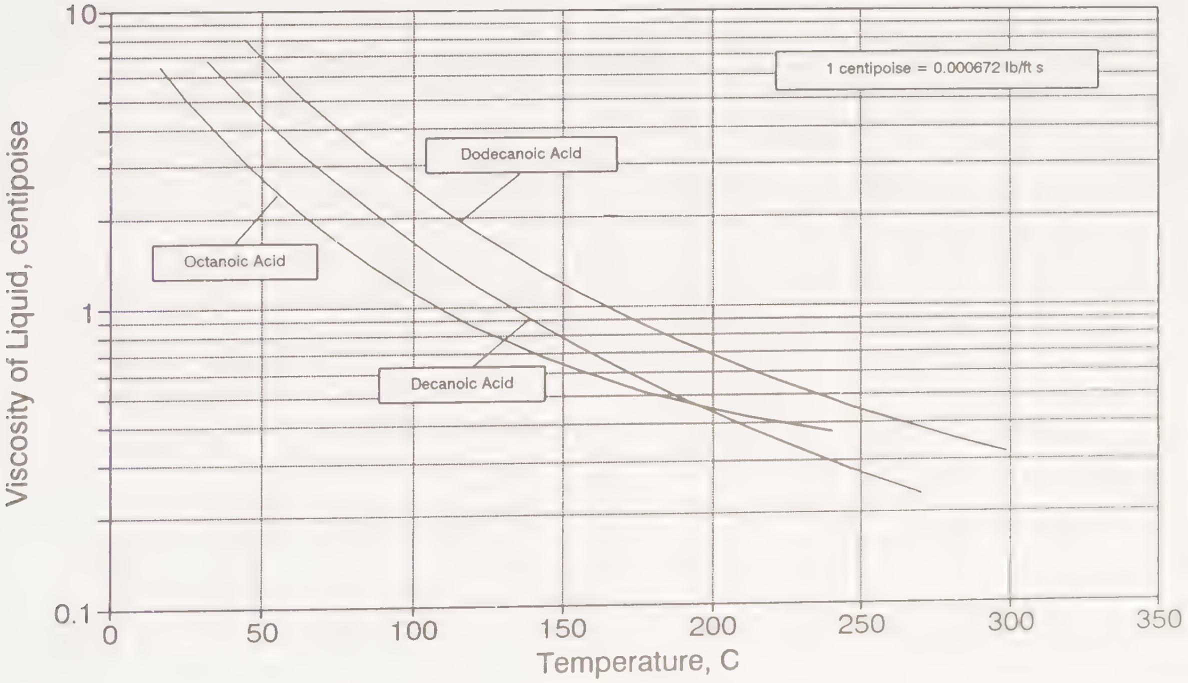

Figure 4-8 Viscosity of Liquid

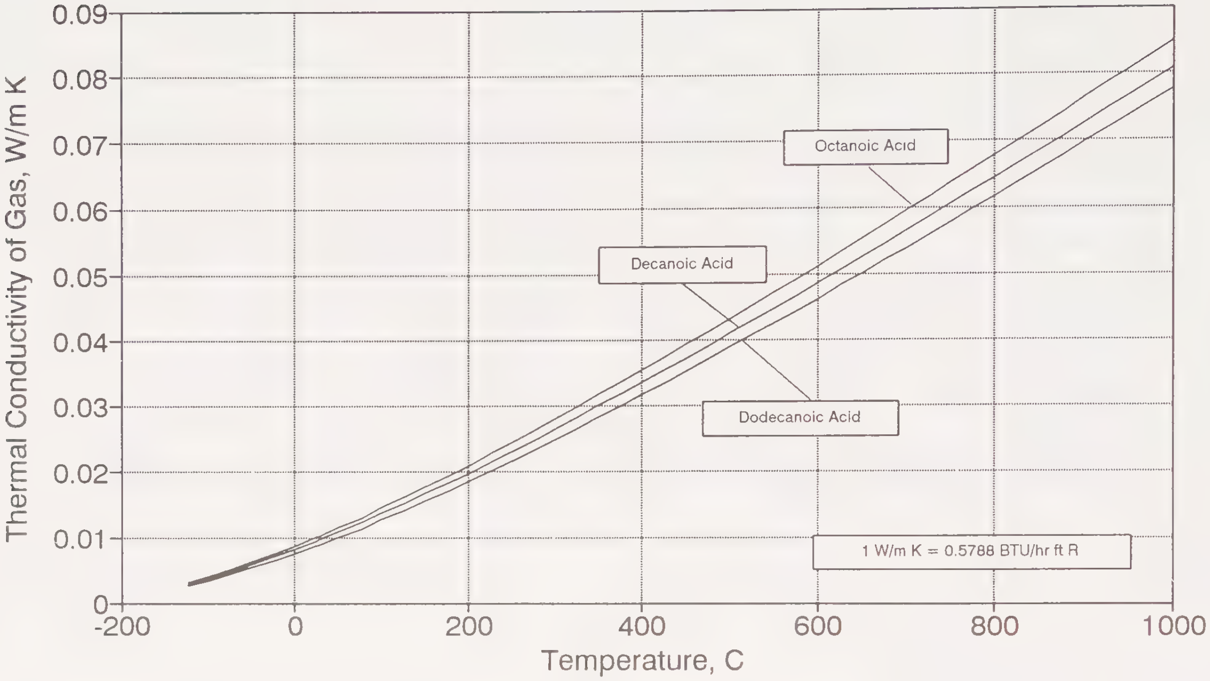

Figure 4-9 Thermal Conductivity of Gas

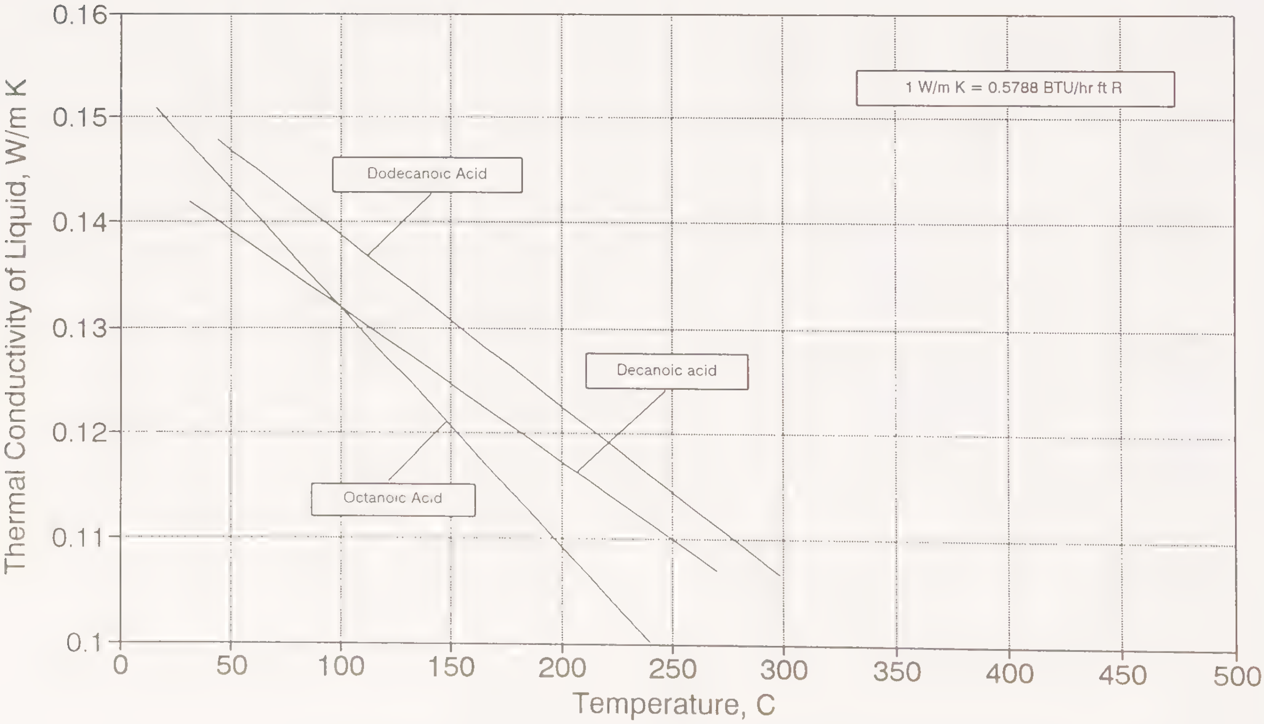

Figure 4-10 Thermal Conductivity of Liquid

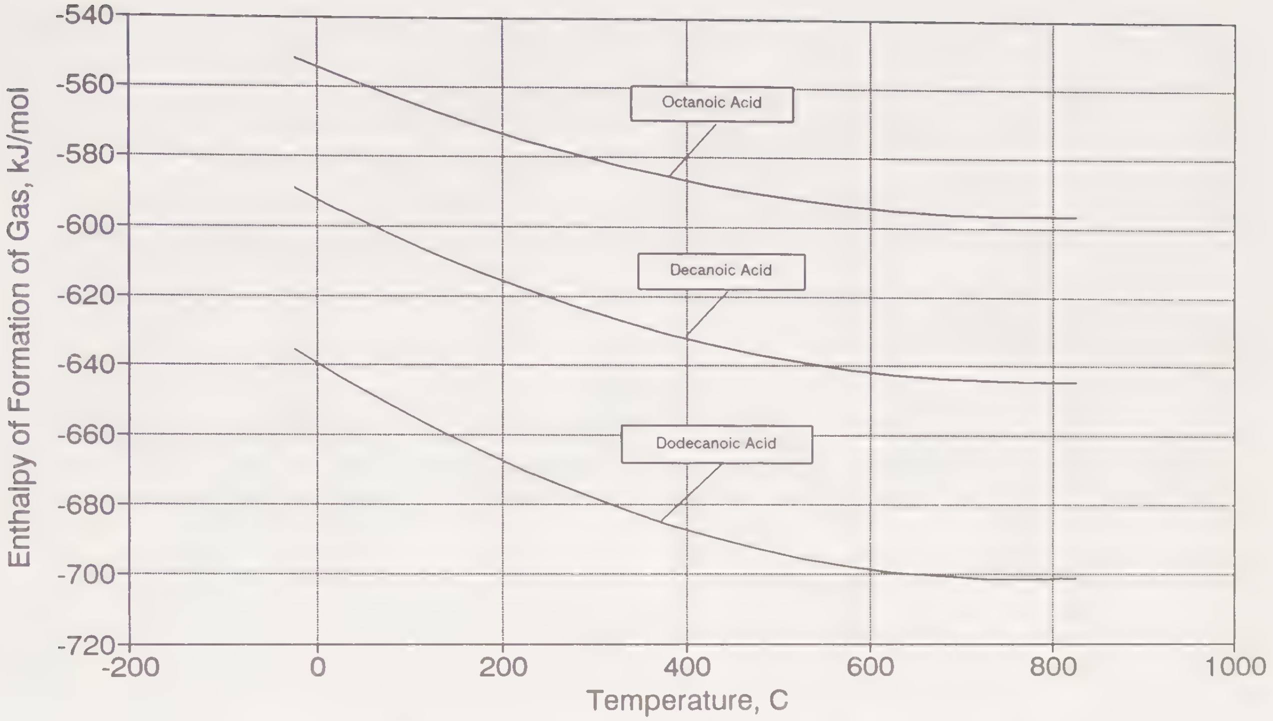

Figure 4-11 Enthalpy of Formation of Gas

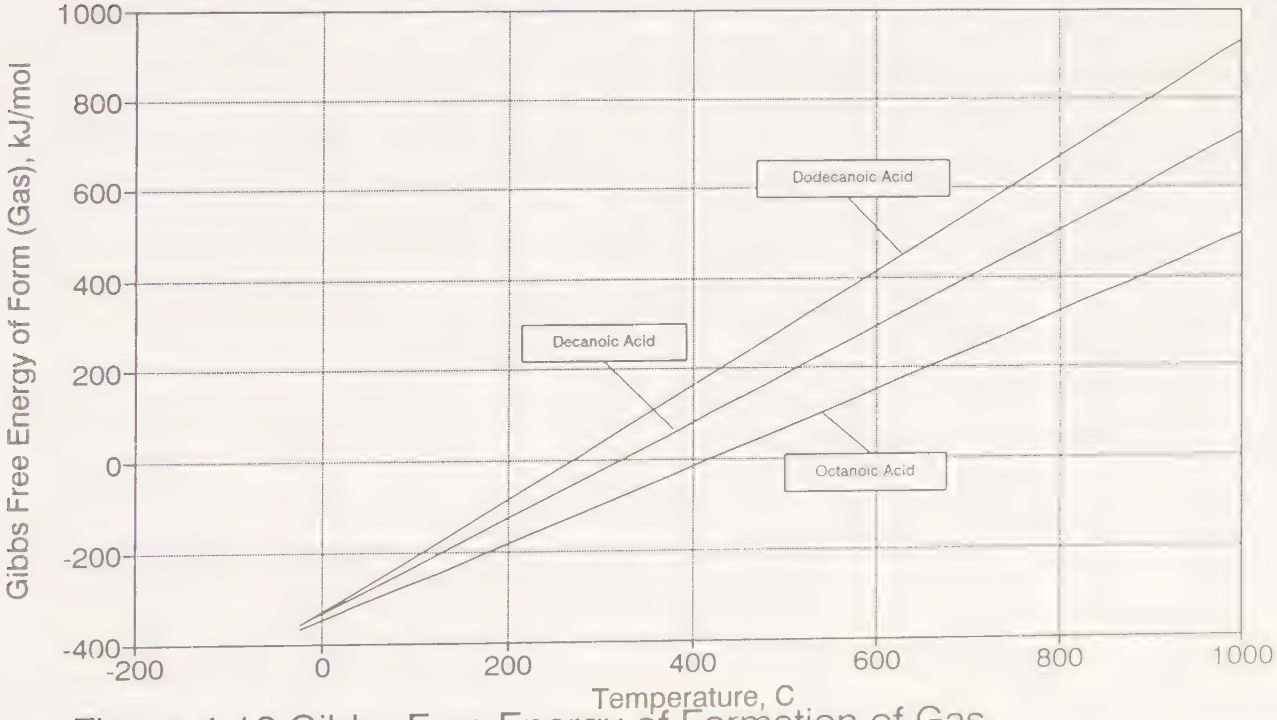

Figure 4-12 Gibbs Free Energy of Formation of Gas

Chapter 5

C_{14}, C_{16} AND C_{18} NORMAL ACIDS

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 5-1

Property data from the literature (2,3,8,21-26,36,63-67,73-79,125-127) are given in Table 5-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available.

VAPOR PRESSURE - Figure 5-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 5-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 5%.

LIQUID DENSITY - Figure 5-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

SURFACE TENSION - Figure 5-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 5-5 and 5-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 5% or less in most cases except for octadecanoic acid (possible 25% error).

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 10% or less in most cases except for tetradecanoic acid (possible 25% error).

VISCOSITY - Figures 5-7 and 5-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 5% or less in most cases.

THERMAL CONDUCTIVITY - Figures 5-9 and 5-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases except for octadecanoic acid (possible 25% error).

ENTHALPY OF FORMATION - Figure 5-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 5-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 5-1 Physical Properties

1. Name	Tetradecanoic Acid	Hexadecanoic Acid	Octadecanoic Acid
2. Formula	C14H28O2	C16H32O2	C18H36O2
3. Molecular Weight, g/mol	228.375	256.429	284.483
4. Critical Temperature, K	756.00	776.00	799.00
5. Critical Pressure, bar	17.000	15.100	13.600
6. Critical Volume, ml/mol	811.00	917.00	1020.00
7. Critical Compressibility Factor	0.219	0.215	0.209
8. Acentric Factor	1.0254	1.0830	1.0841
9. Melting Point, K	327.55	335.95	342.75
10. Boiling Point @ 1 atm, K	599.35	624.15	648.35
11. Heat of Vaporization @ BP, kJ/kg	279.97	255.86	230.90
12. Density of Liquid @ BP, g/ml	0.652	0.631	0.619
13. Surface Tension @ BP, dynes/cm	8.41	8.14	7.92
14. Heat Capacity of Gas @ 25 C, J/g K	1.460	1.479	1.531
15. Heat Capacity of Liquid @ BP, J/g K	3.065	4.324	3.608
16. Viscosity of Gas @ 25 C, micropoise	43.00	40.55	38.31
17. Viscosity of Liquid @ BP, centipoise	0.202	0.309	0.200
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.008	0.008	0.008
19. Thermal Conductivity of Liquid @ BP, W/m K	0.126	0.102	0.078
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-695.61	-738.99	-769.20
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-291.28	-277.73	-248.43
22. Flash Point, K	445.00	453.00	469.00
23. Autoignition Temperture, K	650.00	650.00	668.15
24. Lower Explosion Limit in Air, vol %	0.5	0.5	0.4
25. Upper Explosion Limit in Air, vol %	5.8	4.9	4.9
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

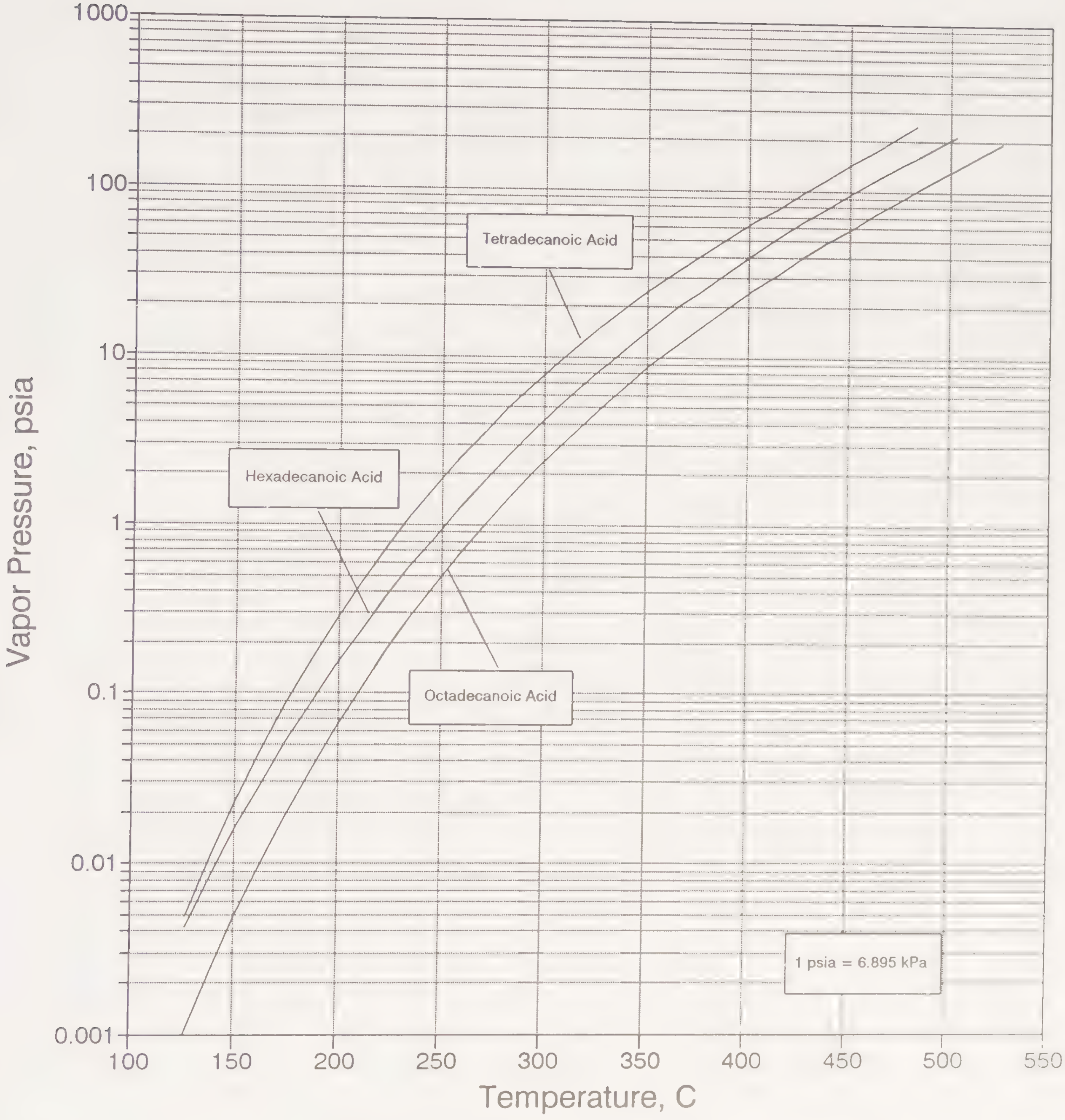

Figure 5-1 Vapor Pressure

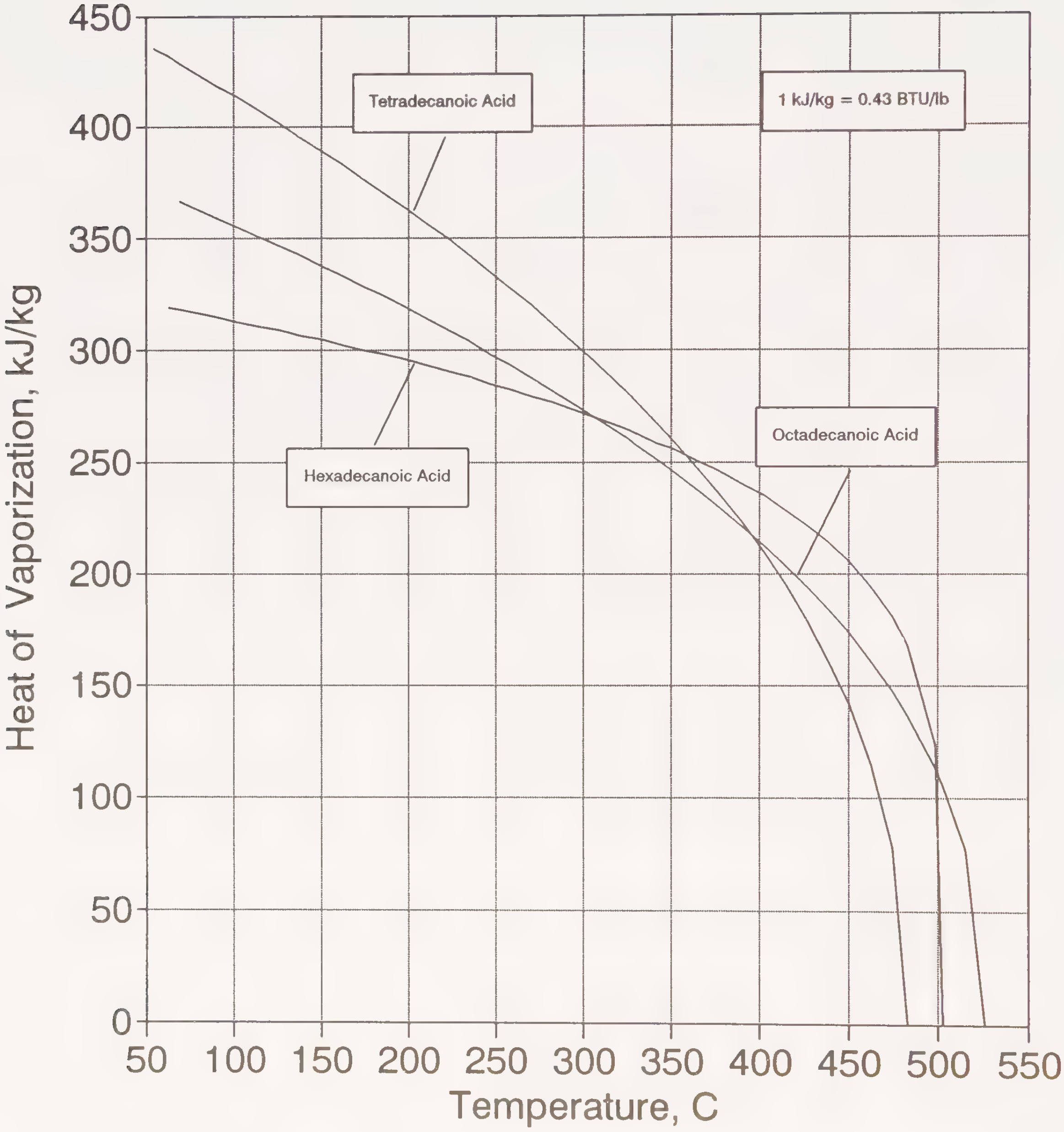

Figure 5-2 Heat of Vaporization

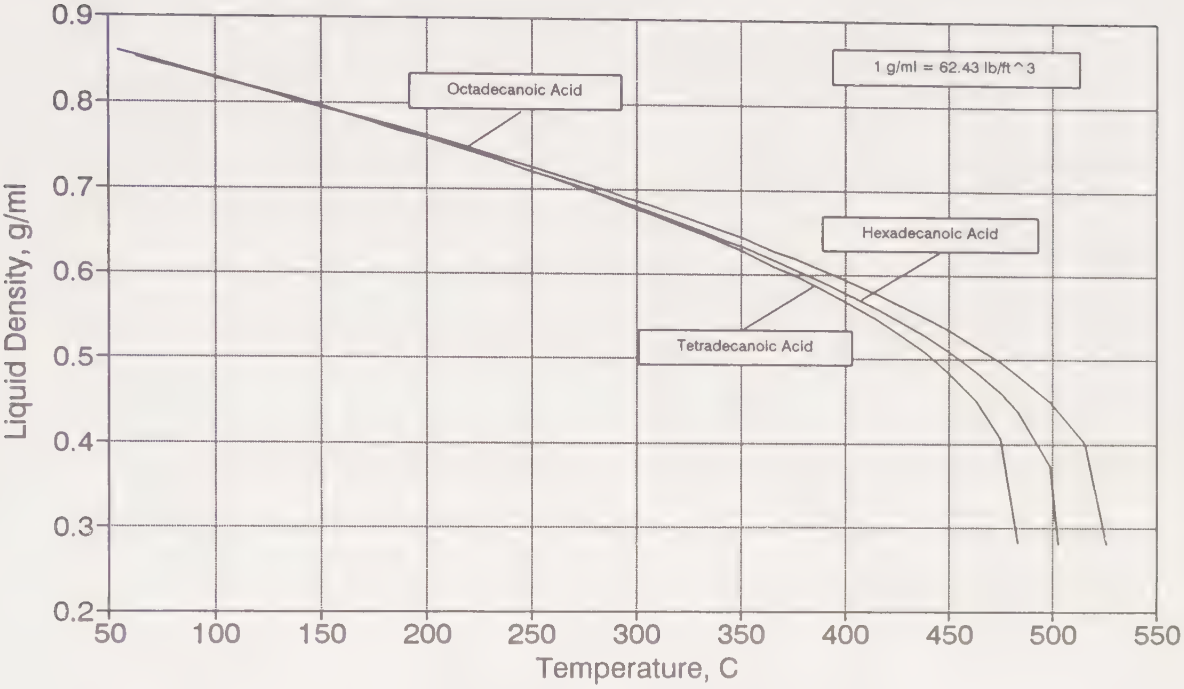

Figure 5-3 Liquid Density

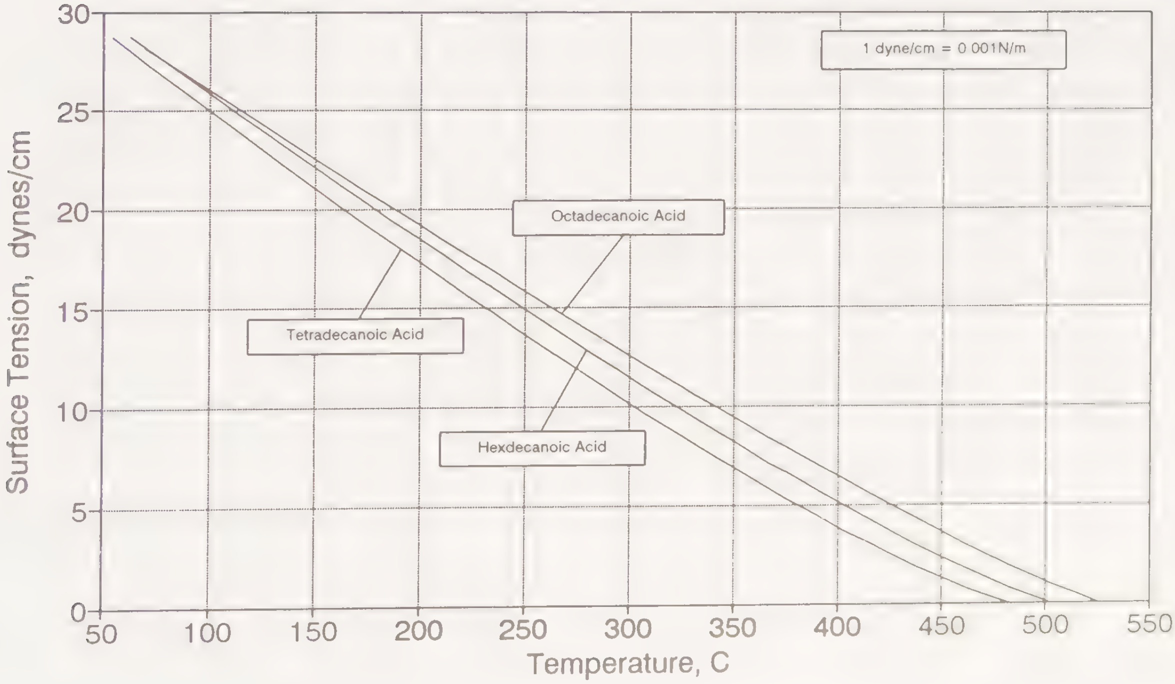

Figure 5-4 Surface Tension

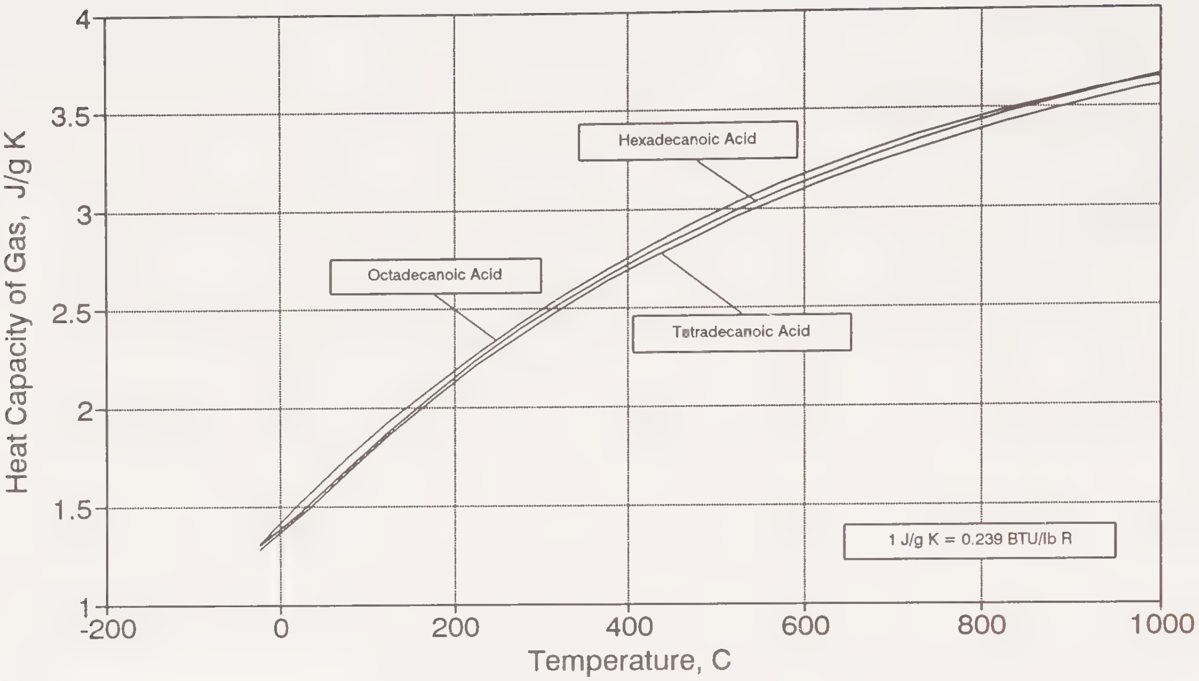

Figure 5-5 Heat Capacity of Gas

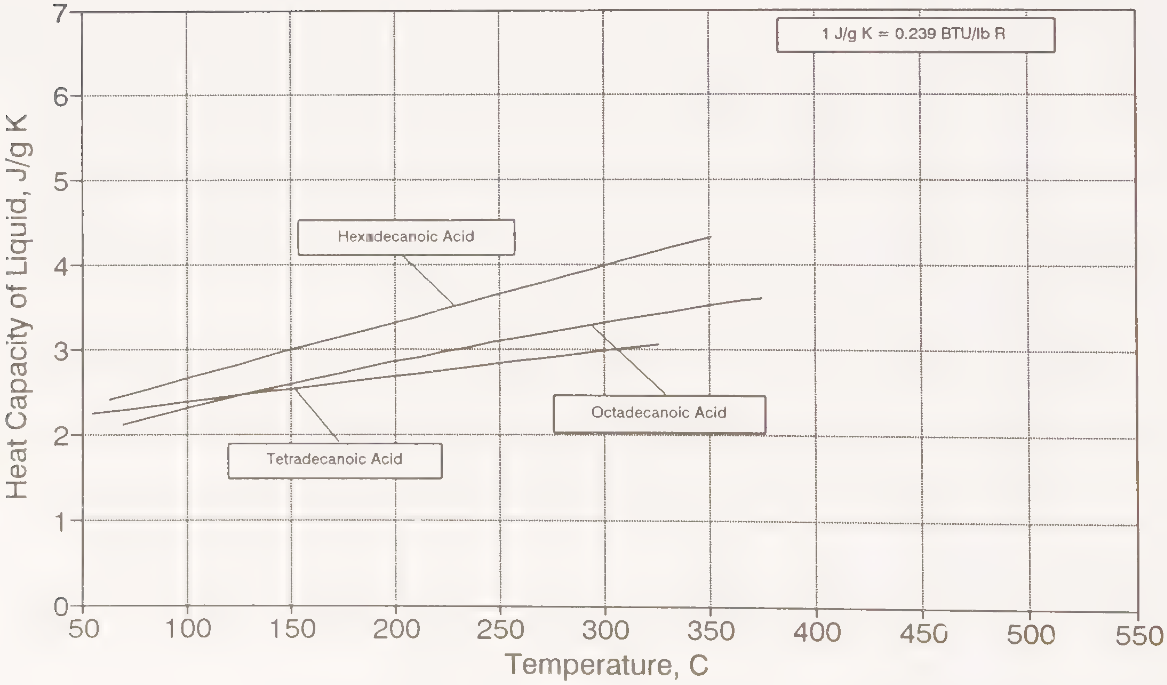

Figure 5-6 Heat Capacity of Liquid

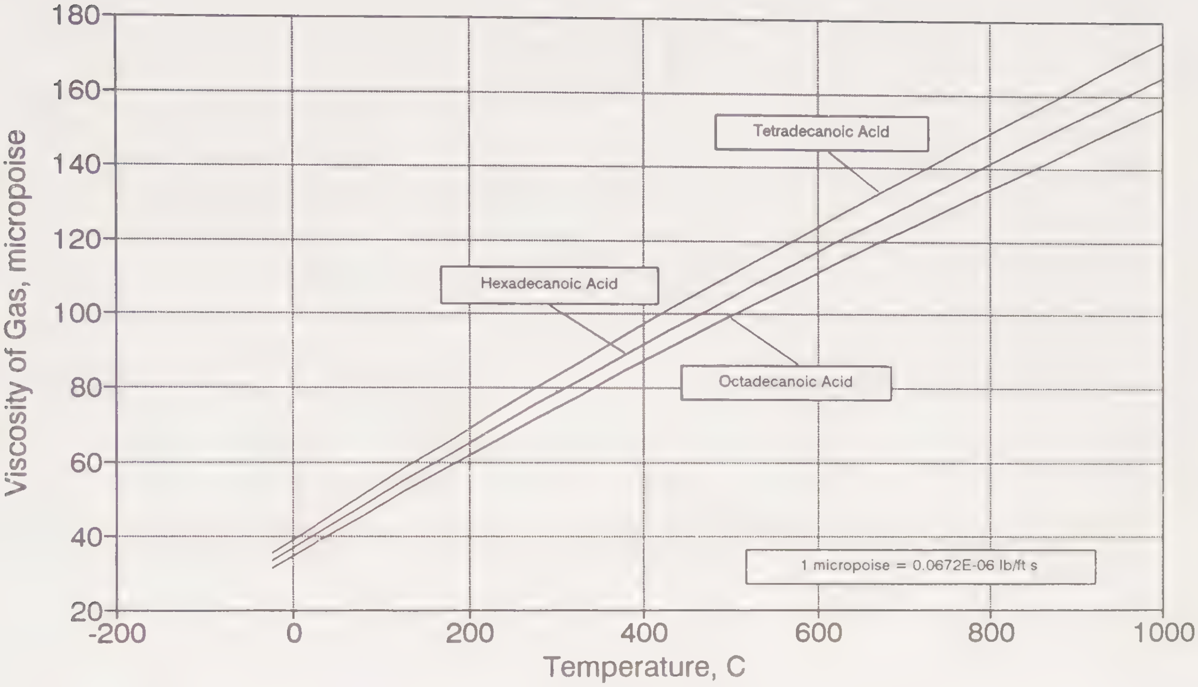

Figure 5-7 Viscosity of Gas

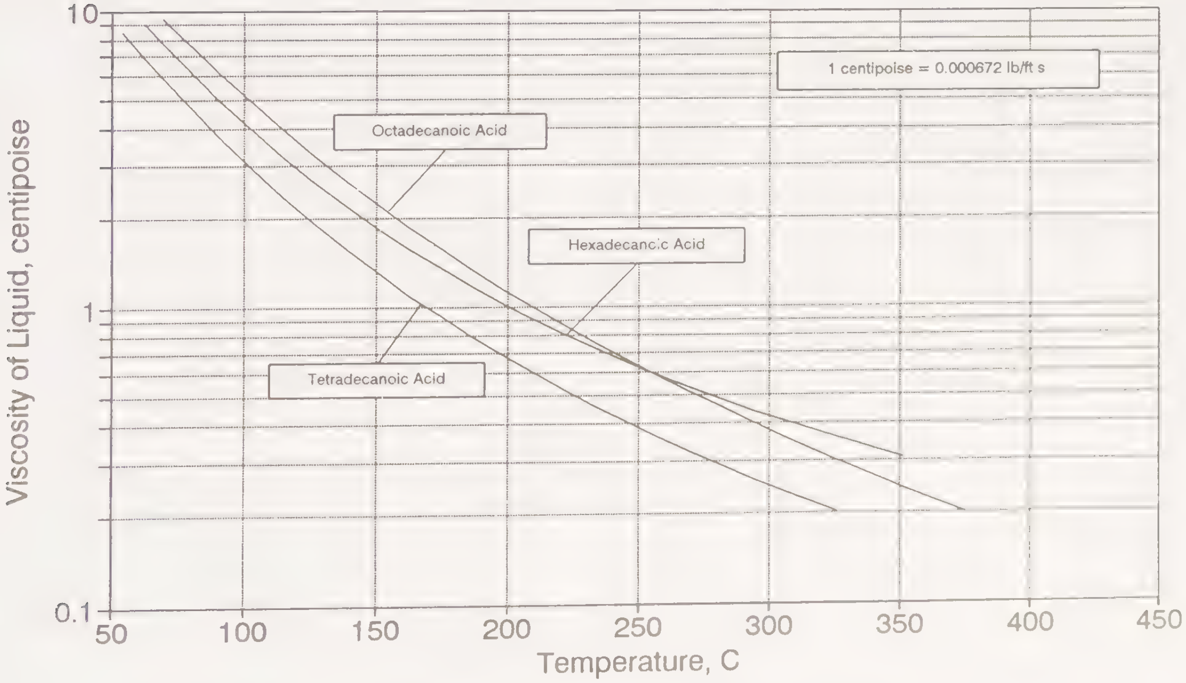

Figure 5-8 Viscosity of Liquid

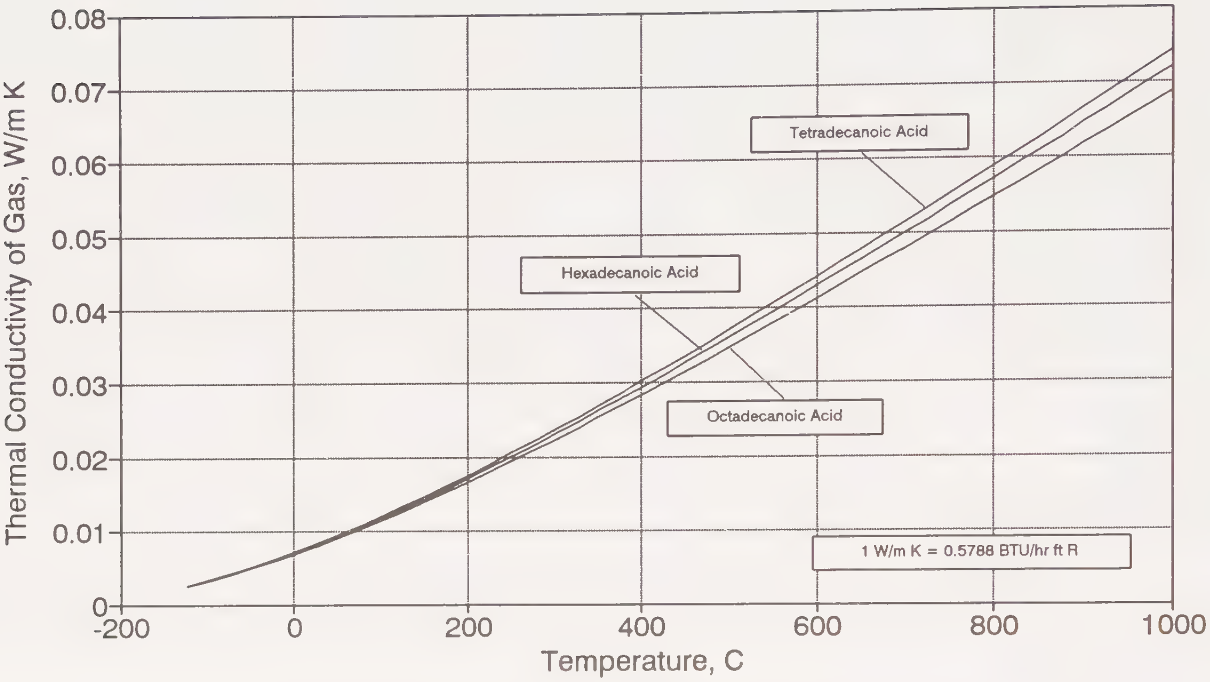

Figure 5-9 Thermal Conductivity of Gas

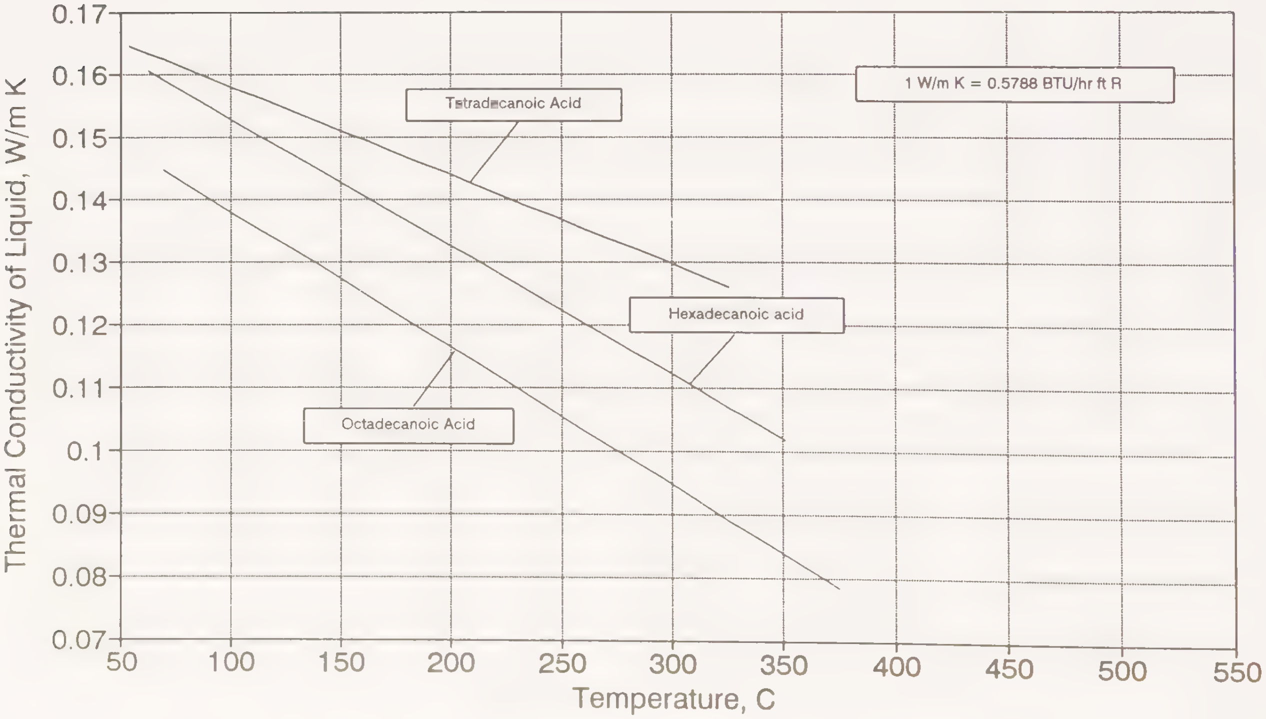

Figure 5-10 Thermal Conductivity of Liquid

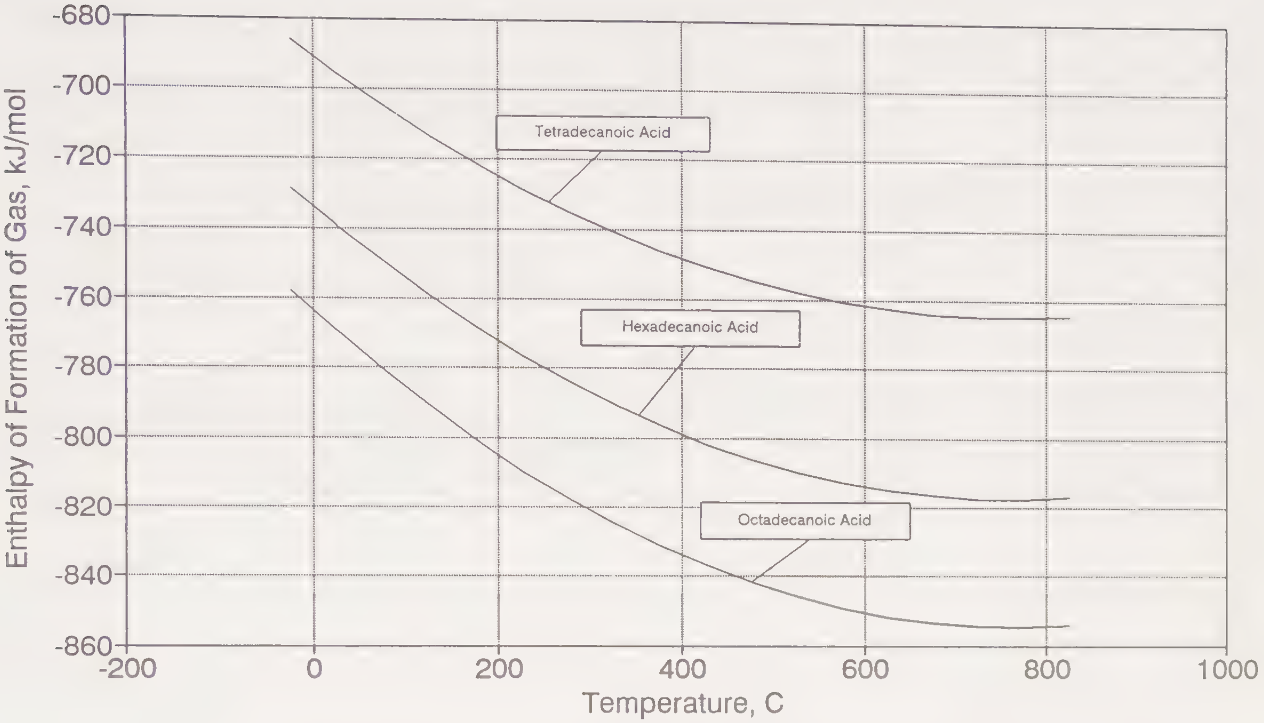

Figure 5-11 Enthalpy of Formation of Gas

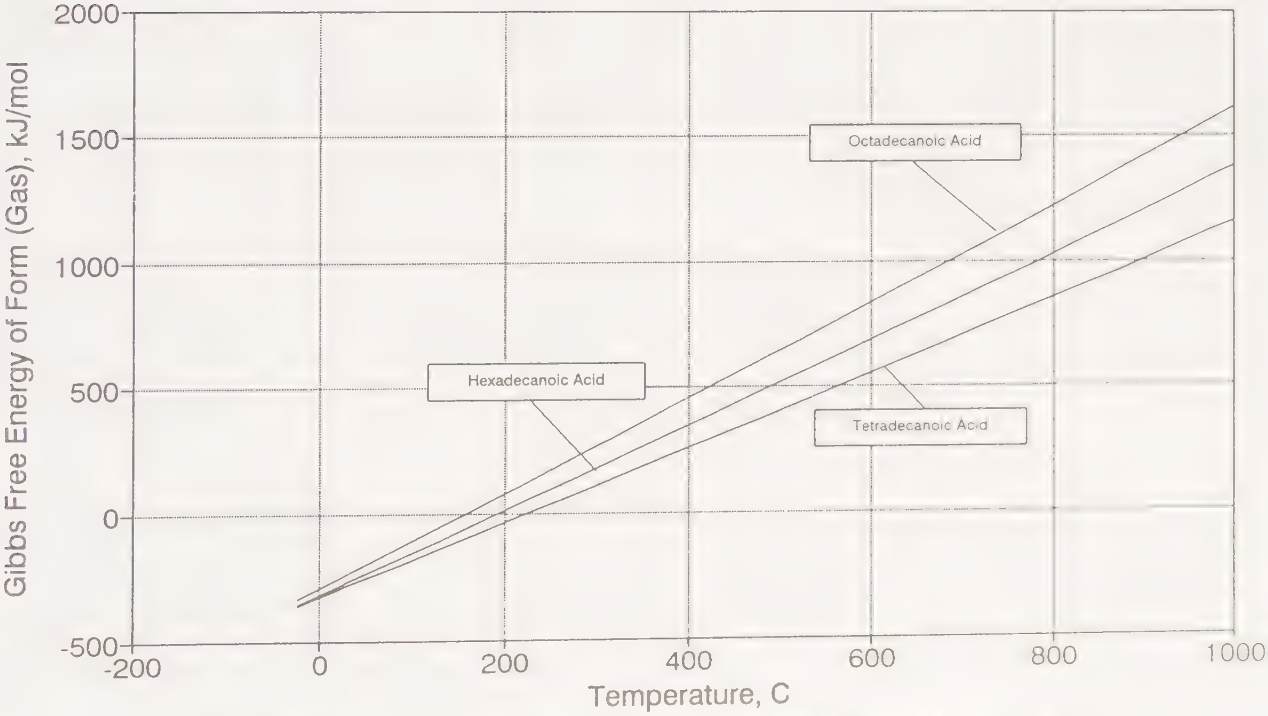

Figure 5-12 Gibbs Free Energy of Formation of Gas

Chapter 6

ADIPIC AND SUCCINIC ACIDS

Robert W. Gallant and Carl L. Yaws

PHYSICAL PROPERTIES - Table 6-1

Property data from the literature (5,9,14,16,25,26,63-65,73,75,79,82,90,93-99) are given in Table 6-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available. References 5, 9 and 26 suggest decomposition reactions at temperatures in the region of the boiling points.

VAPOR PRESSURE - Figure 6-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in rough agreement with experimental data. Errors are about 25% or less in most cases.

HEAT OF VAPORIZATION - Figure 6-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is rough with possible errors of 25%.

LIQUID DENSITY - Figure 6-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in rough agreement with data. Deviations are less than 25% in most cases.

SURFACE TENSION - Figure 6-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 6-5 and 6-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in rough agreement with data. Errors are about 25% or less in most cases.

VISCOSITY - Figures 6-7 and 6-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 10% or less in most cases.

THERMAL CONDUCTIVITY - Figures 6-9 and 6-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 6-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 6-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 6-1 Physical Properties

1. Name	Succinic Acid	Adipic Acid
2. Formula	C4H6O4	C6H10O4
3. Molecular Weight, g/mol	118.089	146.143
4. Critical Temperature, K	806.00	809.00
5. Critical Pressure, bar	47.10	35.30
6. Critical Volume, ml/mol	300.0	400.00
7. Critical Compressibility Factor	0.211	0.210
8. Acentric Factor	0.9914	1.0543
9. Melting Point, K	461.15	425.50
10. Boiling Point @ 1 atm, K	591.00	611.00
11. Heat of Vaporization @ BP, kJ/kg	622.84	499.13
12. Density of Liquid @ BP, g/ml	1.144	0.906
13. Surface Tension @ BP, dynes/cm	27.08	9.68
14. Heat Capacity of Gas @ 25 C, J/g K	1.130	1.170
15. Heat Capacity of Liquid @ BP, J/g K	2.62	3.42
16. Viscosity of Gas @ 25 C, micropoise	63.42	56.57
17. Viscosity of Liquid @ BP, centipoise	0.191	------
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.0099	0.0088
19. Thermal Conductivity of Liquid @ BP, W/m K	0.129	0.117
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-823.49	-866.04
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-697.65	-687.66
22. Flash Point, K	------	435.93
23. Autoignition Temperature, K	------	695.37
24. Lower Explosion Limit in Air, vol %	2.6	1.6
25. Upper Explosion Limit in Air, vol %	14.4	9.6
26. Solubility in Water @ 20 C	6.8%	1.5% @ 15 C

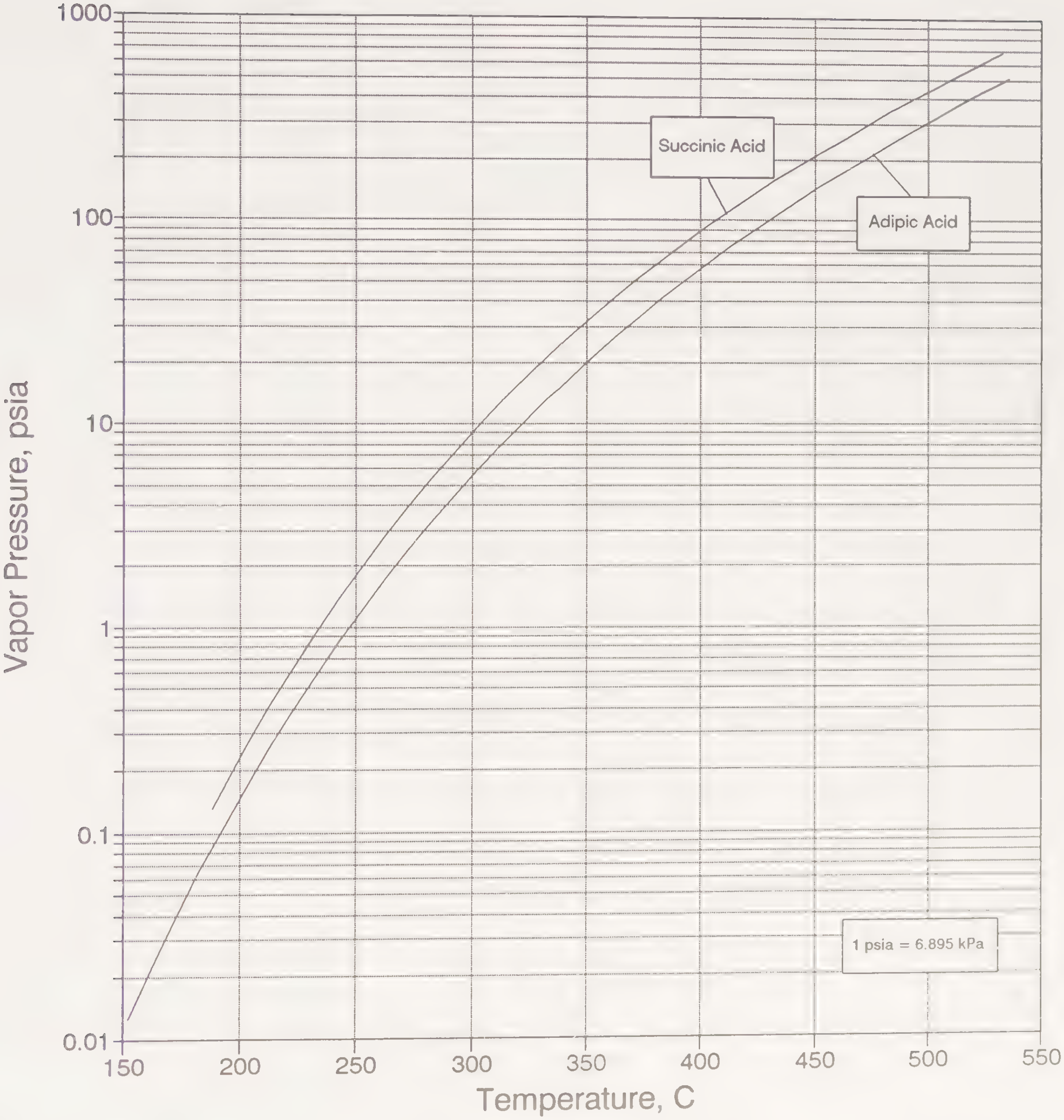

Figure 6-1 Vapor Pressure

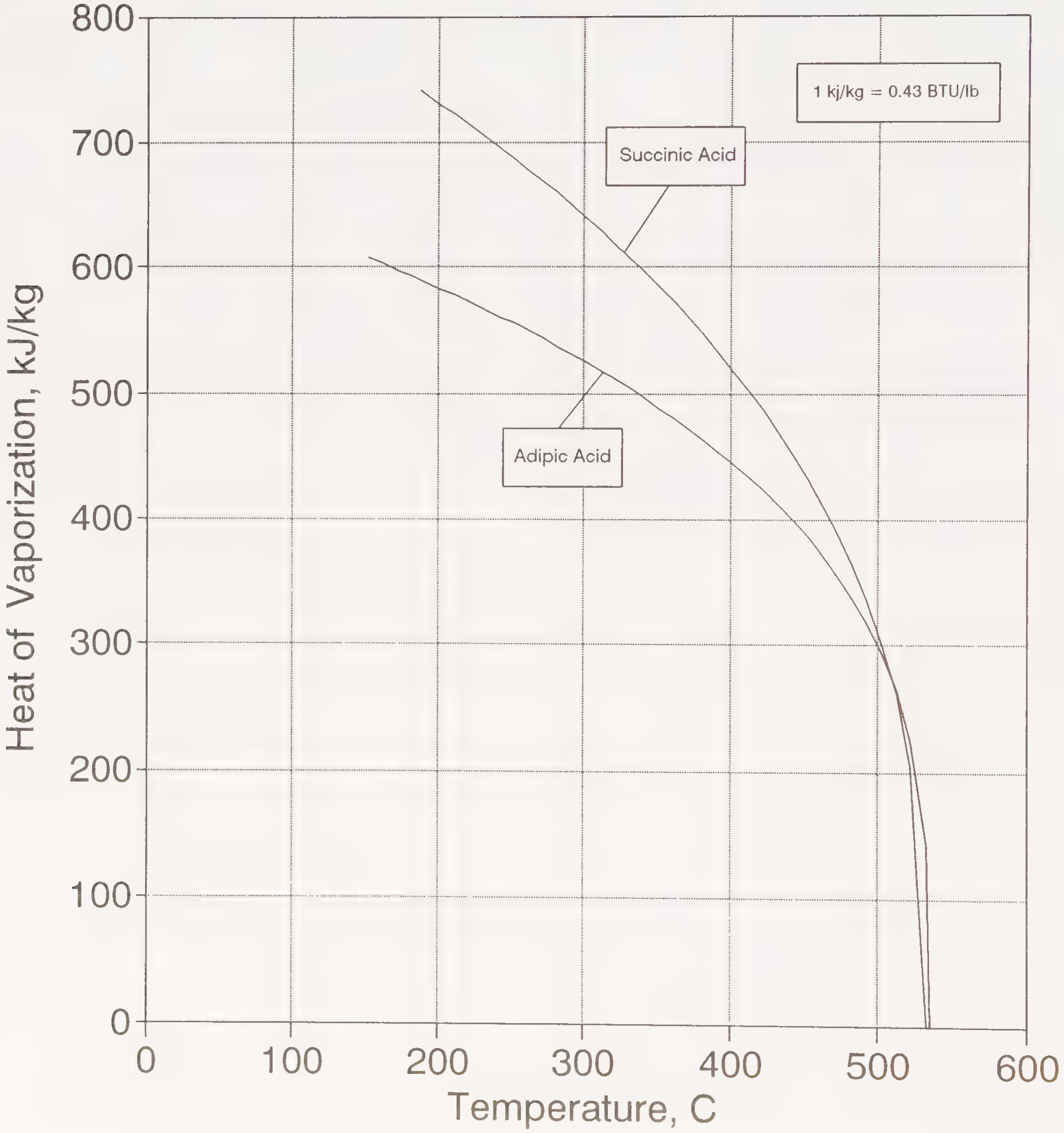

Figure 6-2 Heat of Vaporization

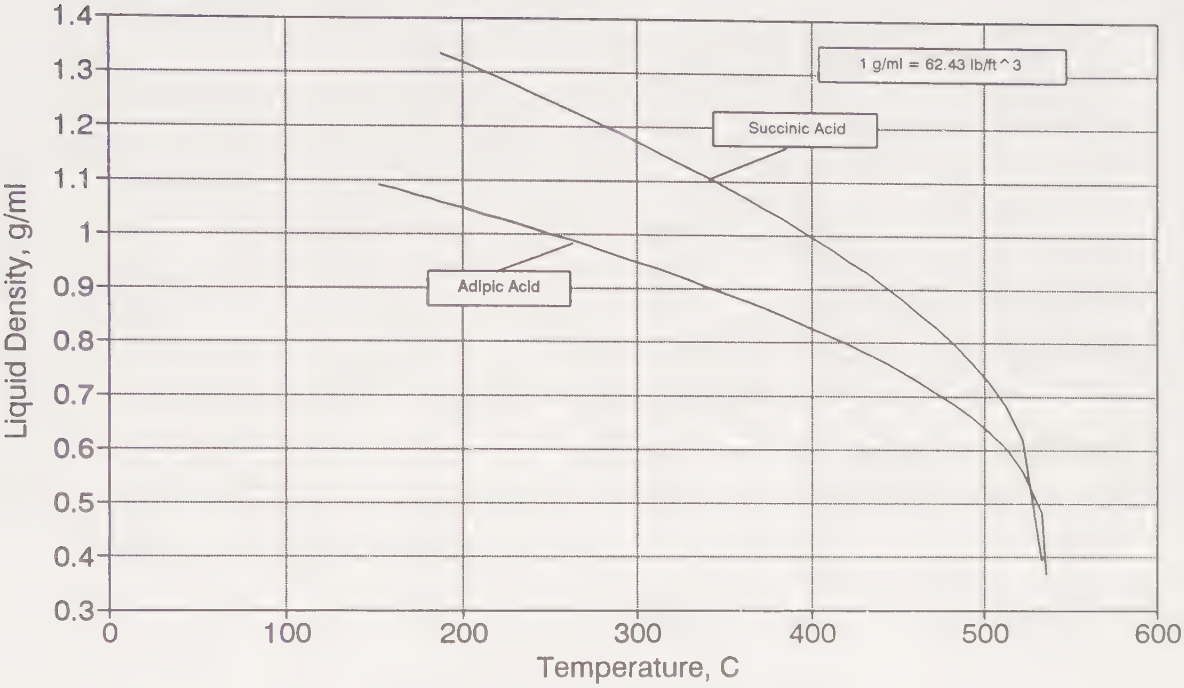

Figure 6-3 Liquid Density

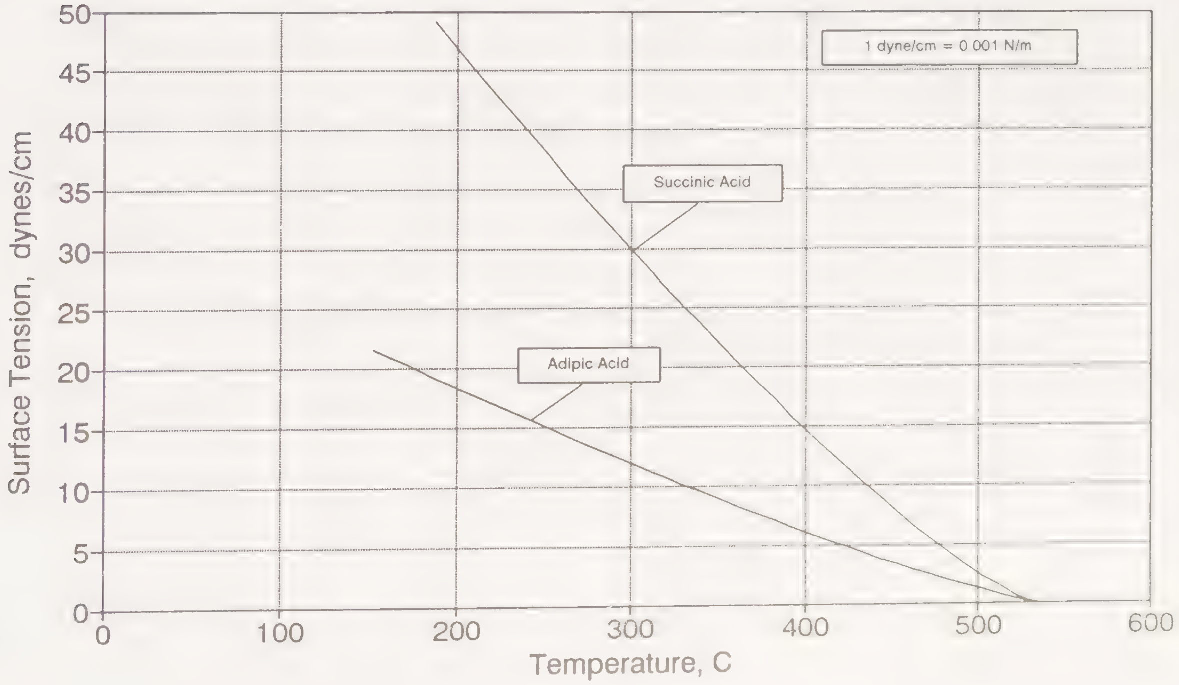

Figure 6-4 Surface Tension

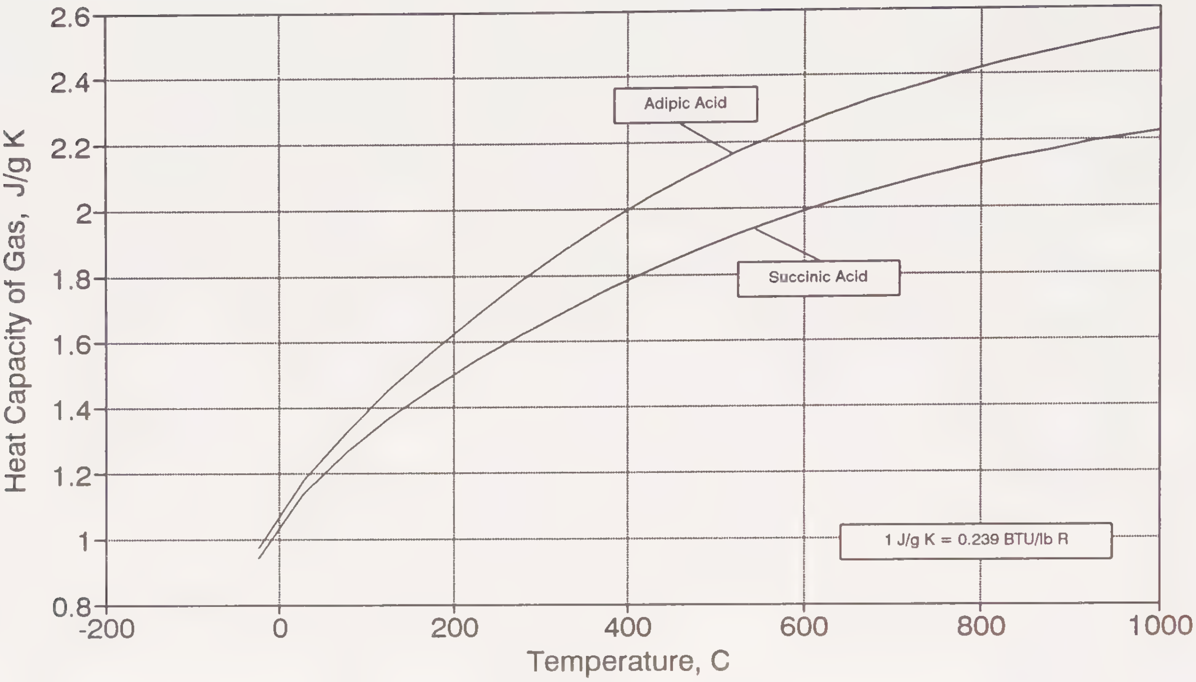

Figure 6-5 Heat Capacity of Gas

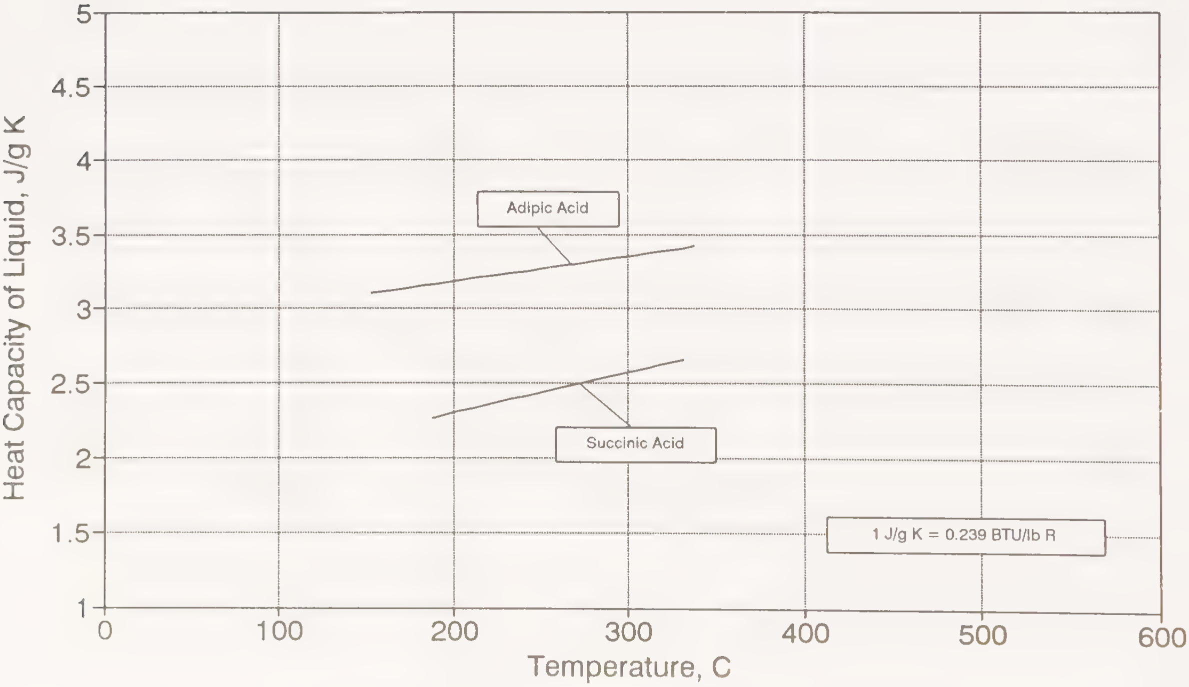

Figure 6-6 Heat Capacity of Liquid

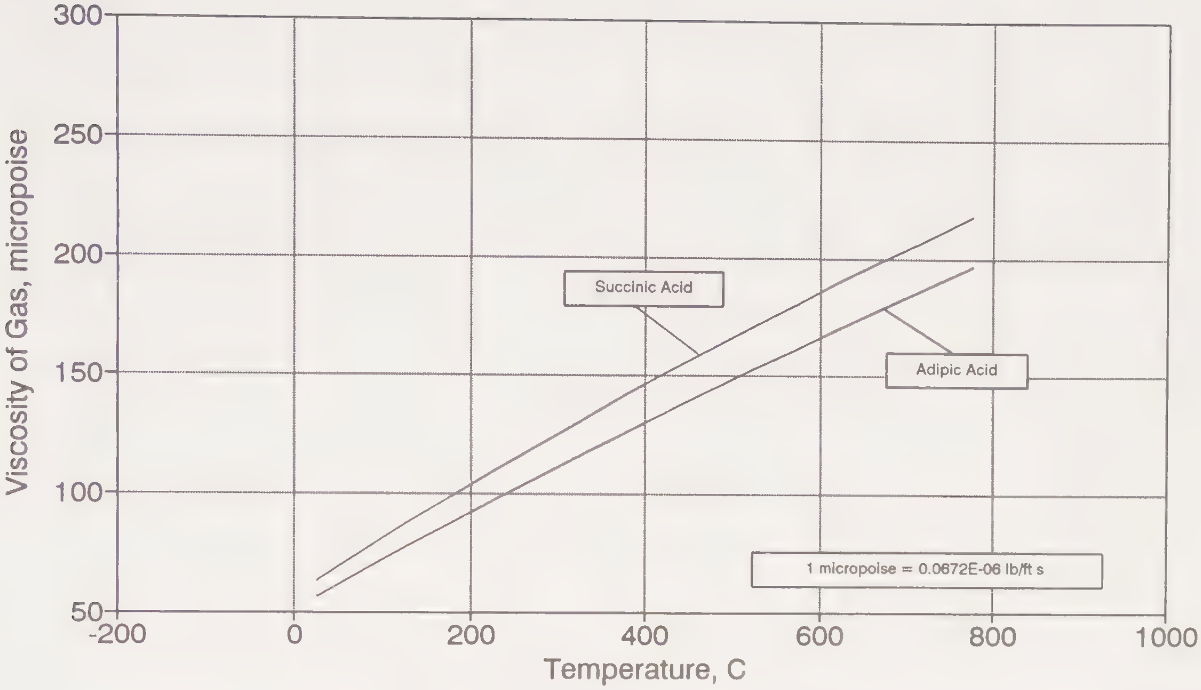

Figure 6-7 Viscosity of Gas

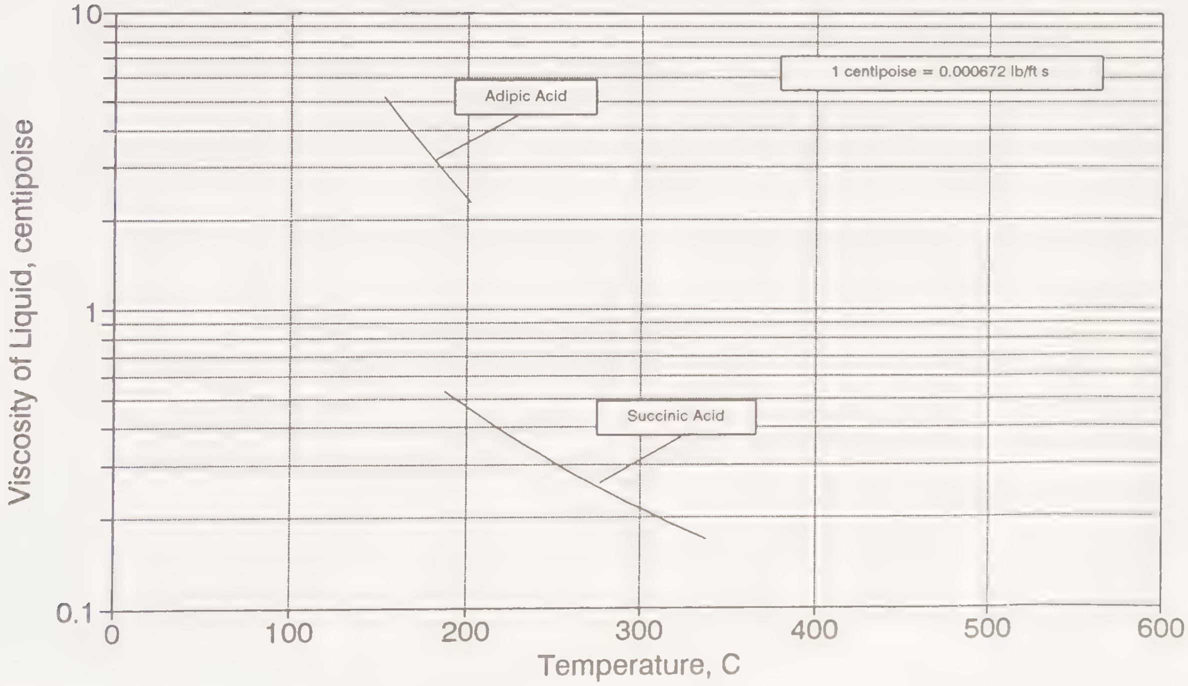

Figure 6-8 Viscosity of Liquid

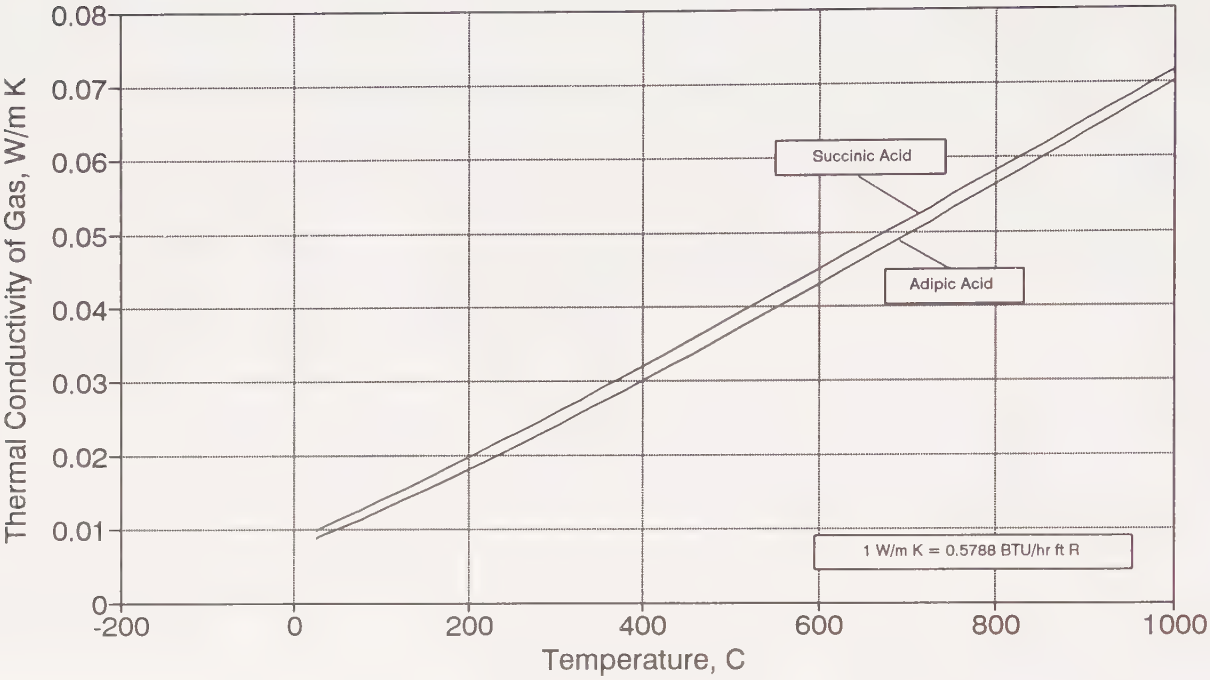

Figure 6-9 Thermal Conductivity of Gas

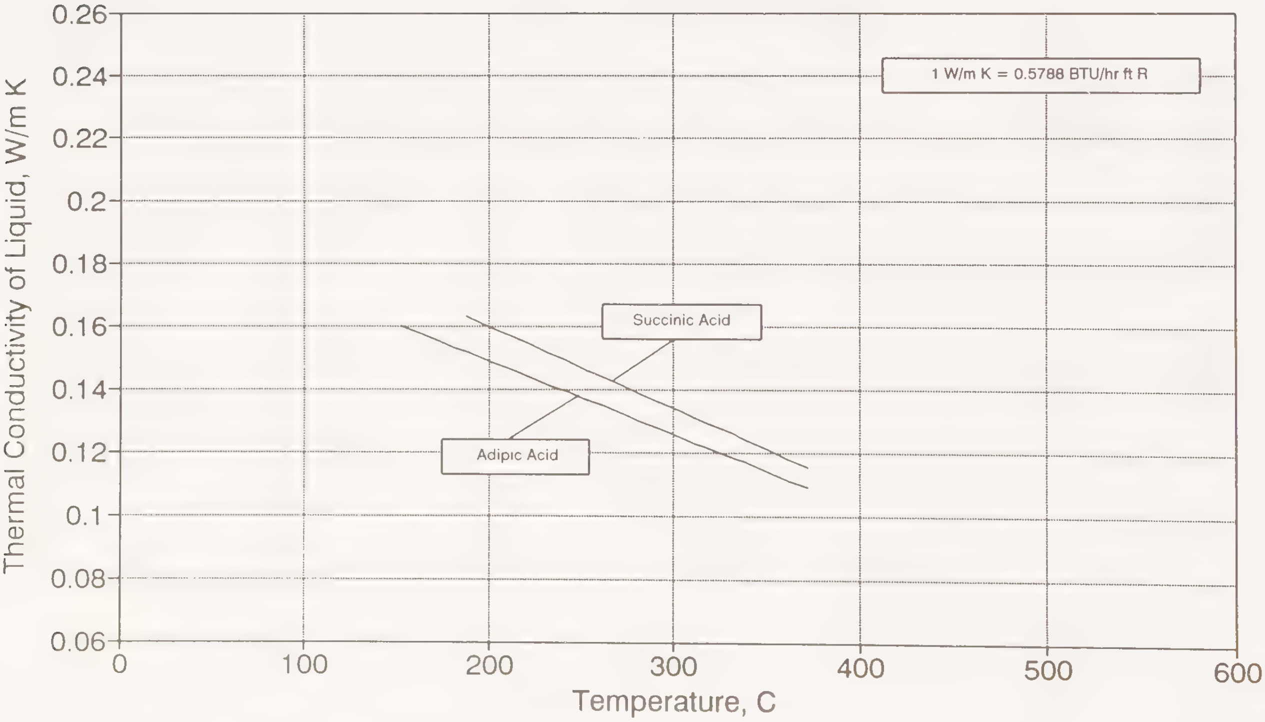

Figure 6-10 Thermal Conductivity of Liquid

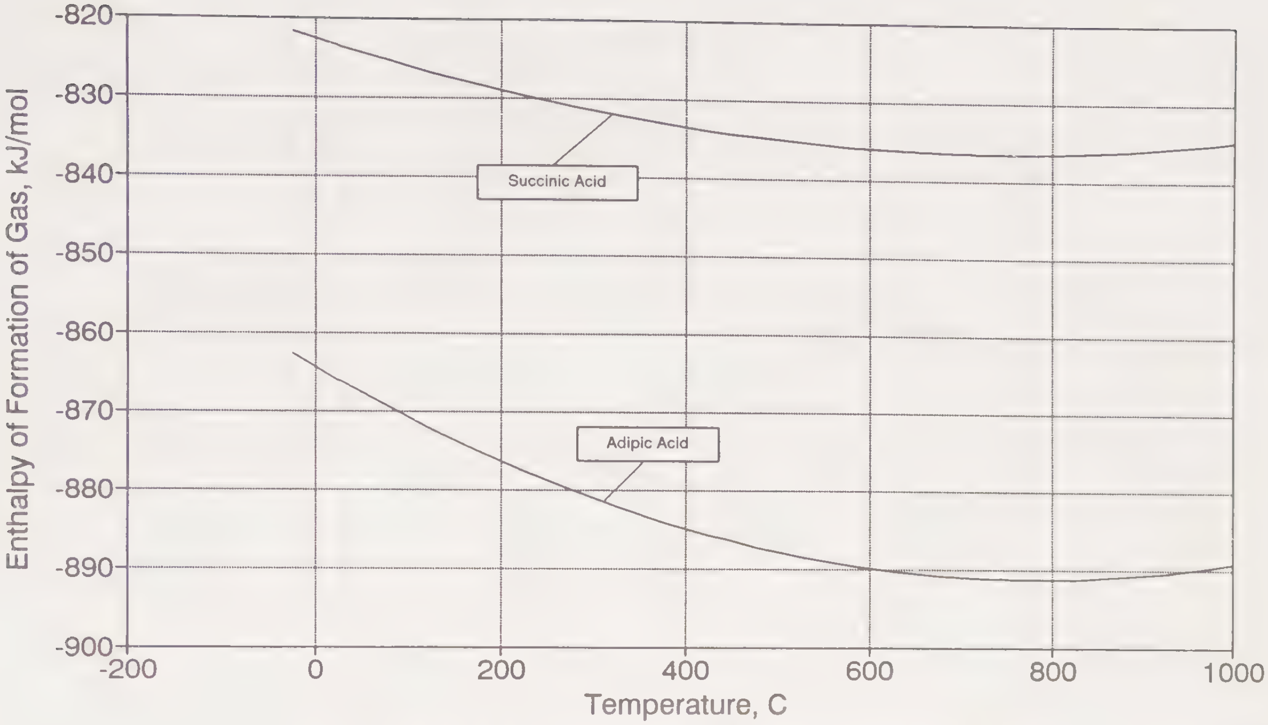

Figure 6-11 Enthalpy of Formation of Gas

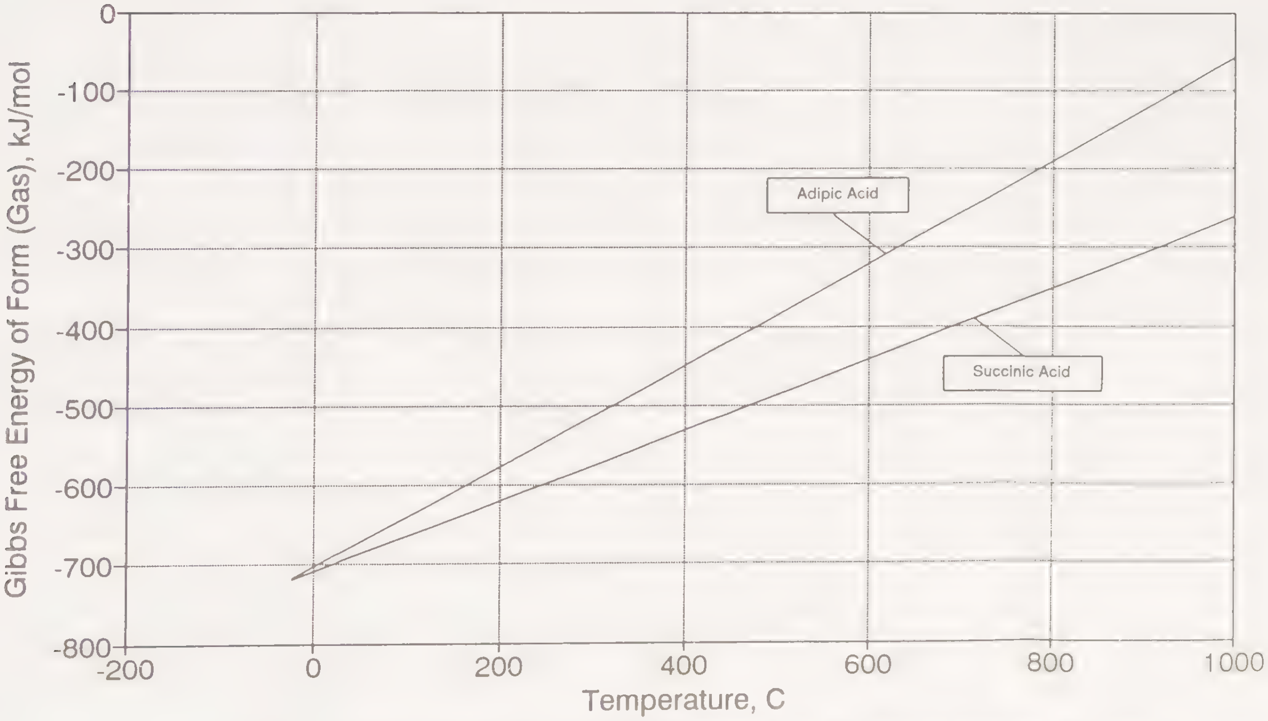

Figure 6-12 Gibbs Free Energy of Formation of Gas

Chapter 7

C_8, C_{10} and C_{12} NORMAL ALCOHOLS

Robert W. Gallant and Carl L. Yaws

PHYSICAL PROPERTIES - Table 7-1

Property data from the literature (2,3,5,6,19,21,26,33,38,44,63-65,73,77,97,100,103-115) are given in Table 7-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available. The DIPPR (Design Institute for Physical Property Research) project (5) and recent data compilations by Yaws and co-workers (44) were consulted extensively in preparing the tabulation.

VAPOR PRESSURE - Figure 7-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 7-2

The data compilation of Yaws and co-workers (44) was selected for heat of vaporization for temperatures ranging from melting point to critical point. The Watson equation, Equation (1-2a), was used for correlation of the data as a function of temperature. Reliability of results is good with errors of about 10% or less.

LIQUID DENSITY - Figure 7-3

Results from the data compilation of Yaws and co-workers (44) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. A modified Rackett equation, Equation (1-3a), was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 2% in most cases.

SURFACE TENSION - Figure 7-4

The data compilation of Yaws and co-workers (44) was selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by the modified Othmer equation, Equation (1-4a). Accuracy is good with errors being about 3% or less in most cases.

HEAT CAPACITY - Figures 7-5 and 7-6

Results from the data compilation of Yaws and co-workers (44) were selected for heat capacity of ideal gas. Correlation of data was accomplished using a series expansion in temperature, Equation (1-5b). Results are in favorable agreement with data. Errors are about 1% or less in most cases.

Results from the data compilation of Yaws and co-workers (44) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6a). Results are in favorable agreement with data. Errors are about 10% or less using the correlation.

VISCOSITY - Figures 7-7 and 7-8

The DIPPR project (5) was selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in favorable agreement with data. Errors are about 10% or less in most cases.

The DIPPR project (5) was also selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 10% or less.

THERMAL CONDUCTIVITY - Figures 7-9 and 7-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using the Equation (1-9). Reliability of results is good with errors of about 10% or less in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Results are in favorable agreement with data. Errors are about 5% or less in most cases.

ENTHALPY OF FORMATION - Figure 7-11

The data compilation of Yaws and co-workers (44) was selected for enthalpy of formation of ideal gas. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 7-12

Results from the data compilation of Yaws and co-workers (44) were selected for Gibb's free energy of formation of ideal gas. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Correlation results are in favorable agreement with data.

Table 7-1 Physical Properties

1. Name	Octanol	Decanol	Dodecanol
2. Formula	C8H18O	C10H22O	C12H26O
3. Molecular Weight, g/mol	130.23	158.284	186.338
4. Critical Temperature, K	652.50	690.00	721.00
5. Critical Pressure, bar	28.60	23.70	19.30
6. Critical Volume, ml/mol	490.0	599.56	696.00
7. Critical Compressibility Factor	0.258	0.248	0.224
8. Acentric Factor	0.5944	0.6134	0.6393
9. Melting Point, K	257.65	280.05	296.95
10. Boiling Point @ 1 atm, K	468.35	503.35	535.00
11. Heat of Vaporization @ BP, kJ/kg	388.70	317.69	361.92
12. Density of Liquid @ 25 C, g/ml	0.822	0.827	0.842
13. Surface Tension @ 25 C, dynes/cm	27.04	28.44	29.40
14. Heat Capacity of Gas @ 25 C, J/g K	1.546	1.561	1.572
15. Heat Capacity of Liquid @ 25 C, J/g K	1.974	1.967	1.925
16. Viscosity of Gas @ 25 C, micropoise	53.98	50.36	44.50
17. Viscosity of Liquid @ 25 C, centipoise	7.29	11.32	15.72
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.010	0.010	0.011
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.161	0.162	0.146
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-357.29	-403.44	-443.15
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-117.99	-106.27	-87.95
22. Flash Point, K	354.26	355.37	399.82
23. Autoignition Temperture, K	555.0	561.15	548.15
24. Lower Explosion Limit in Air, vol %	0.9	0.7	0.6
25. Upper Explosion Limit in Air, vol %	6.4	5.5	5.1
26. Solubility in Water @ 25 C, ppm(wt)	540.00	37.02	4.00

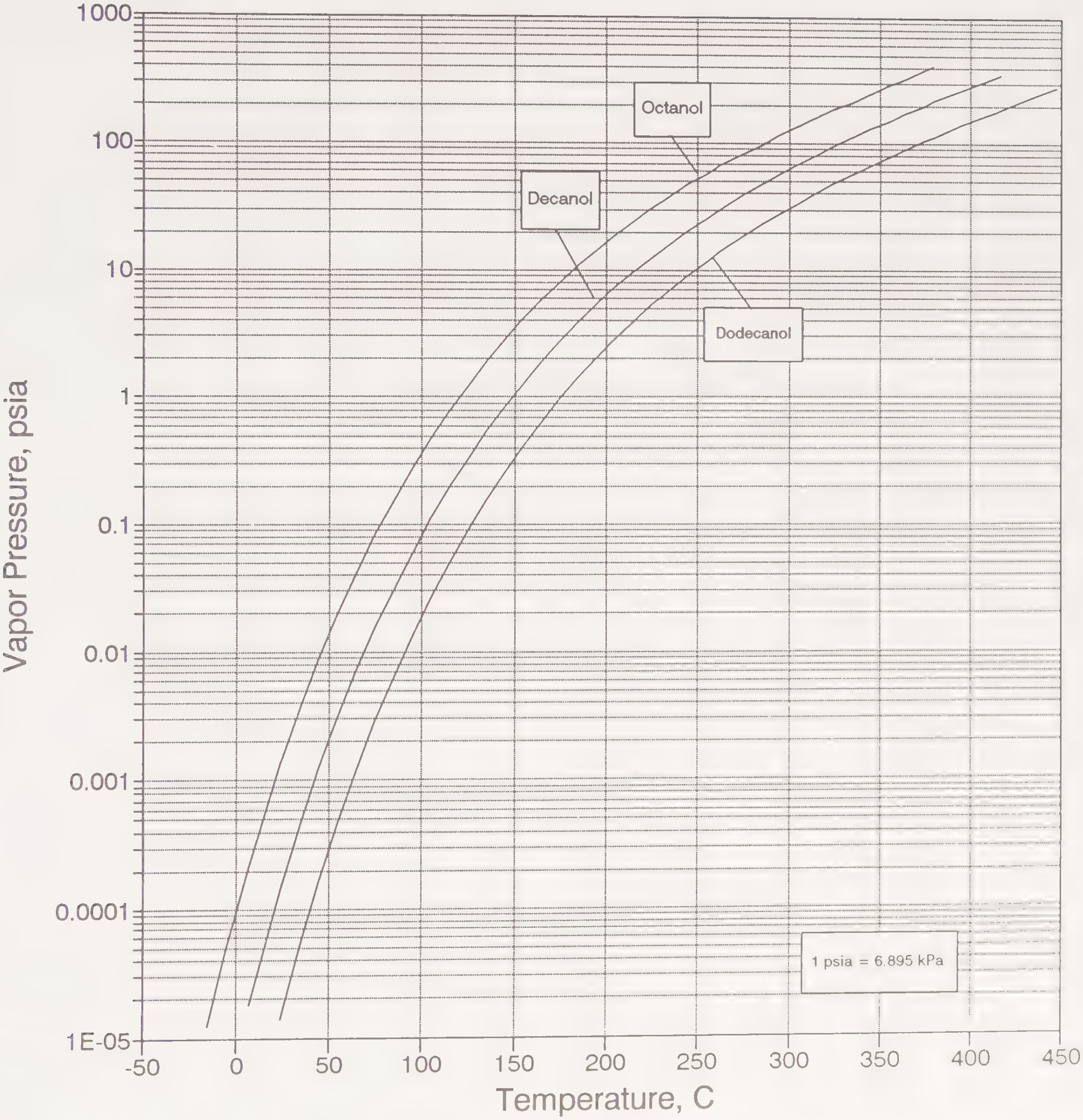

Figure 7-1 Vapor Pressure

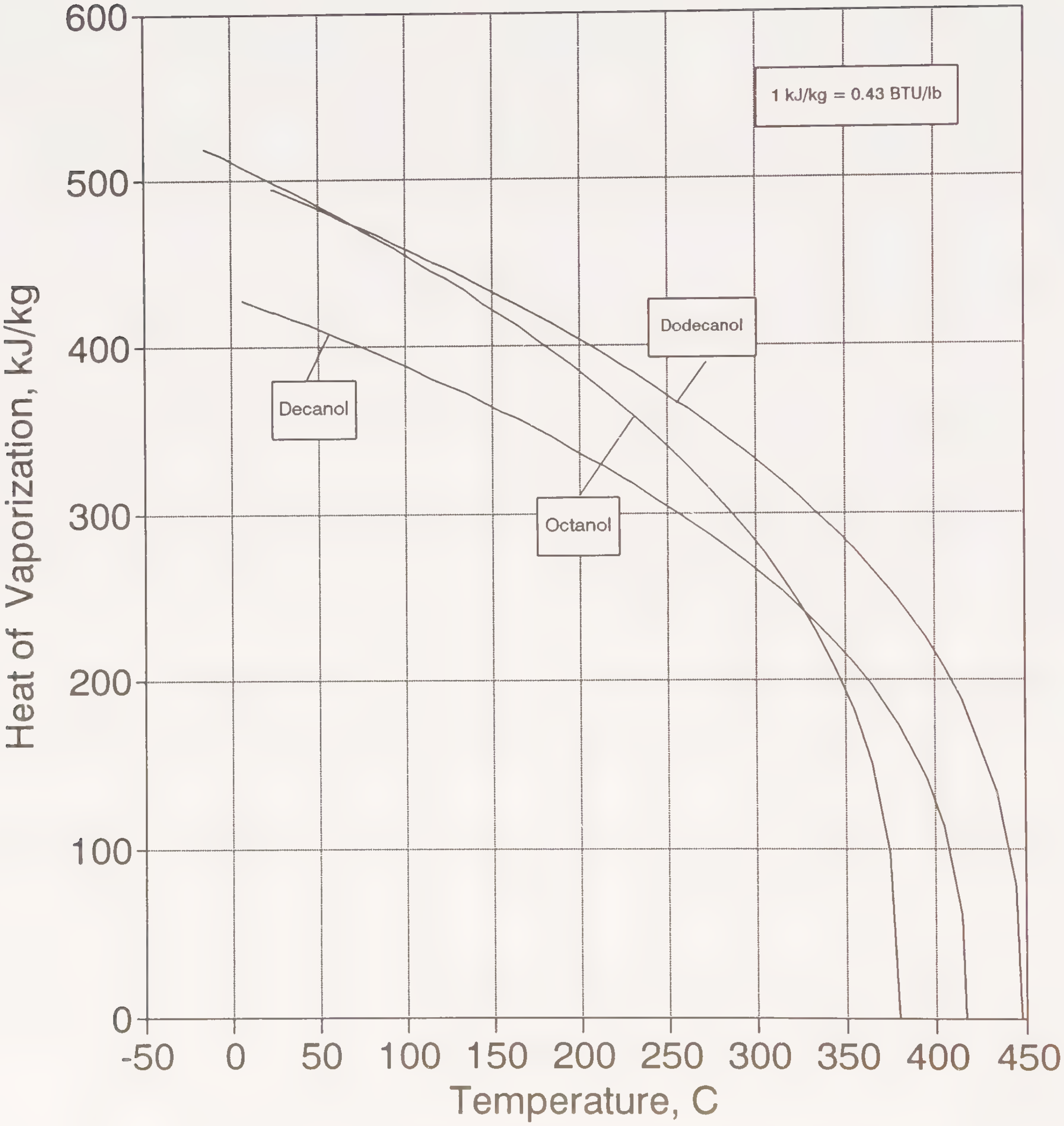

Figure 7-2 Heat of Vaporization

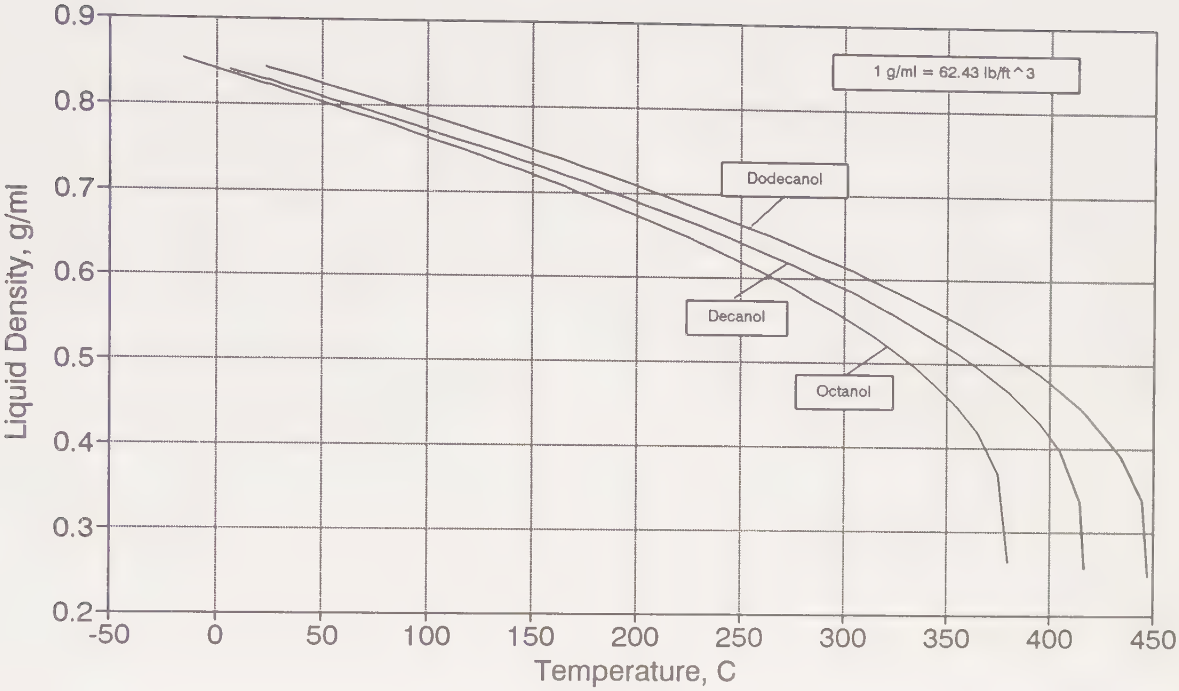

Figure 7-3 Liquid Density

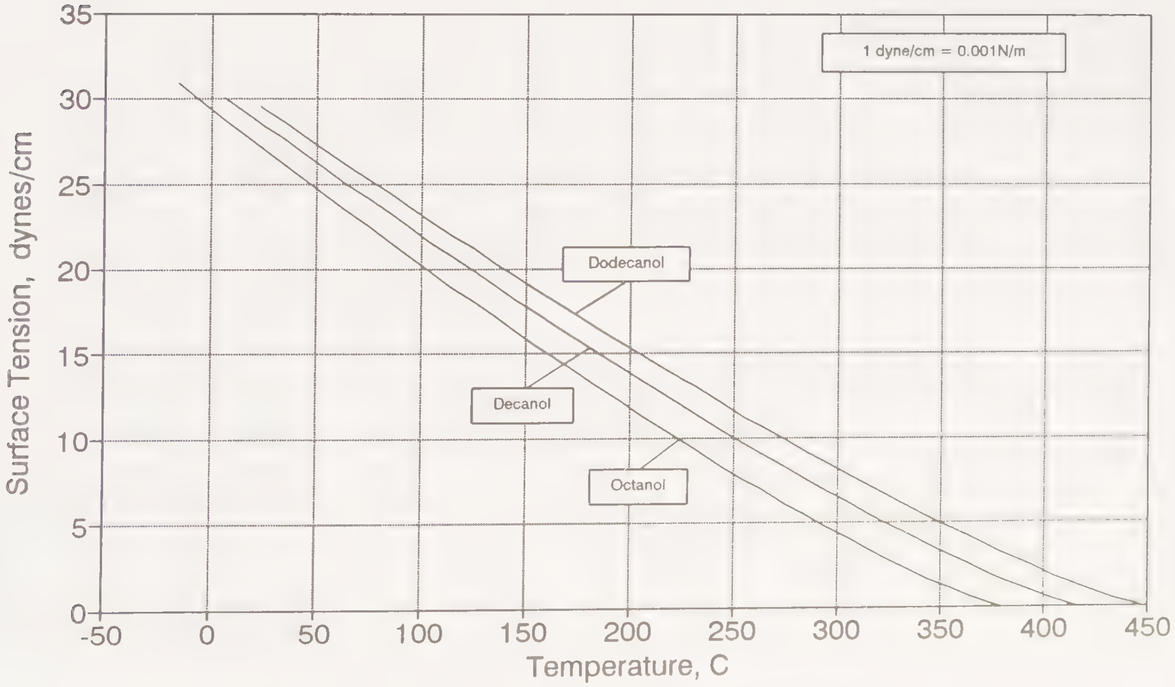

Figure 7-4 Surface Tension

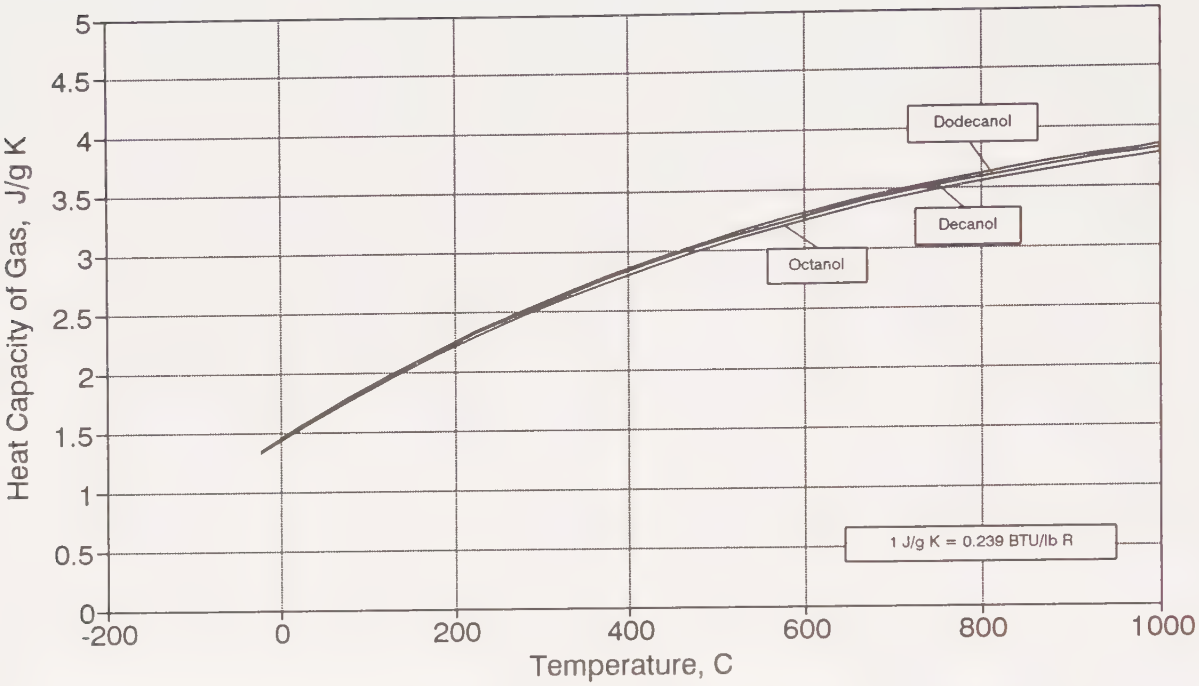

Figure 7-5 Heat Capacity of Gas

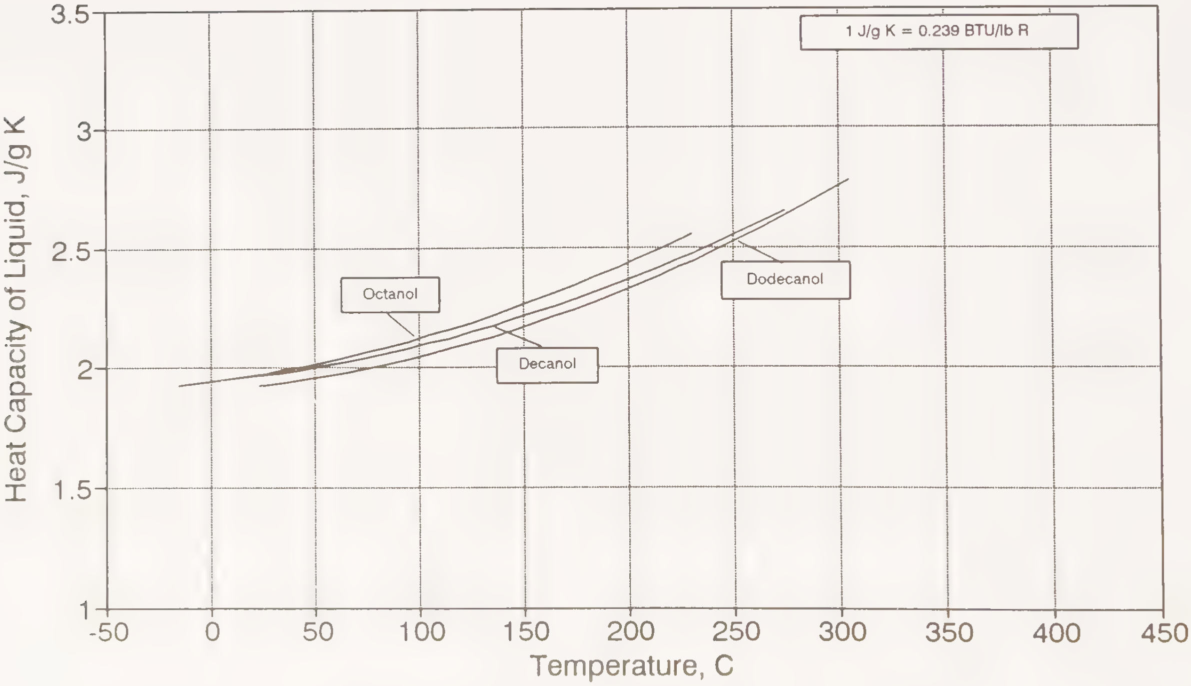

Figure 7-6 Heat Capacity of Liquid

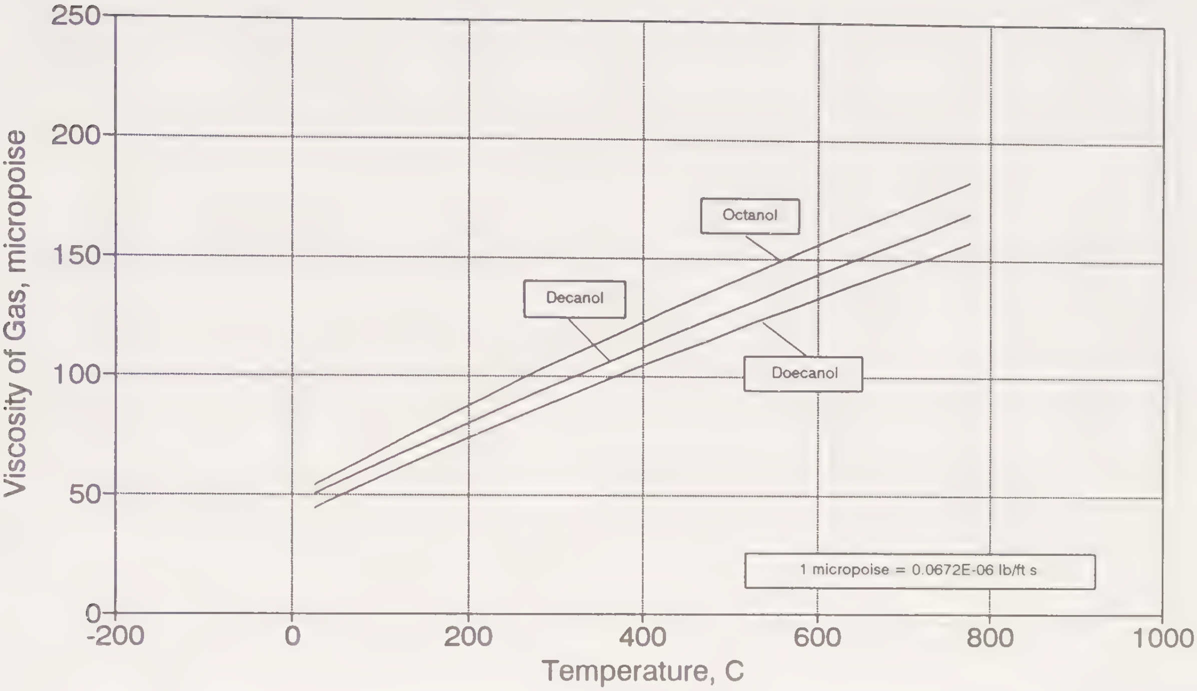

Figure 7-7 Viscosity of Gas

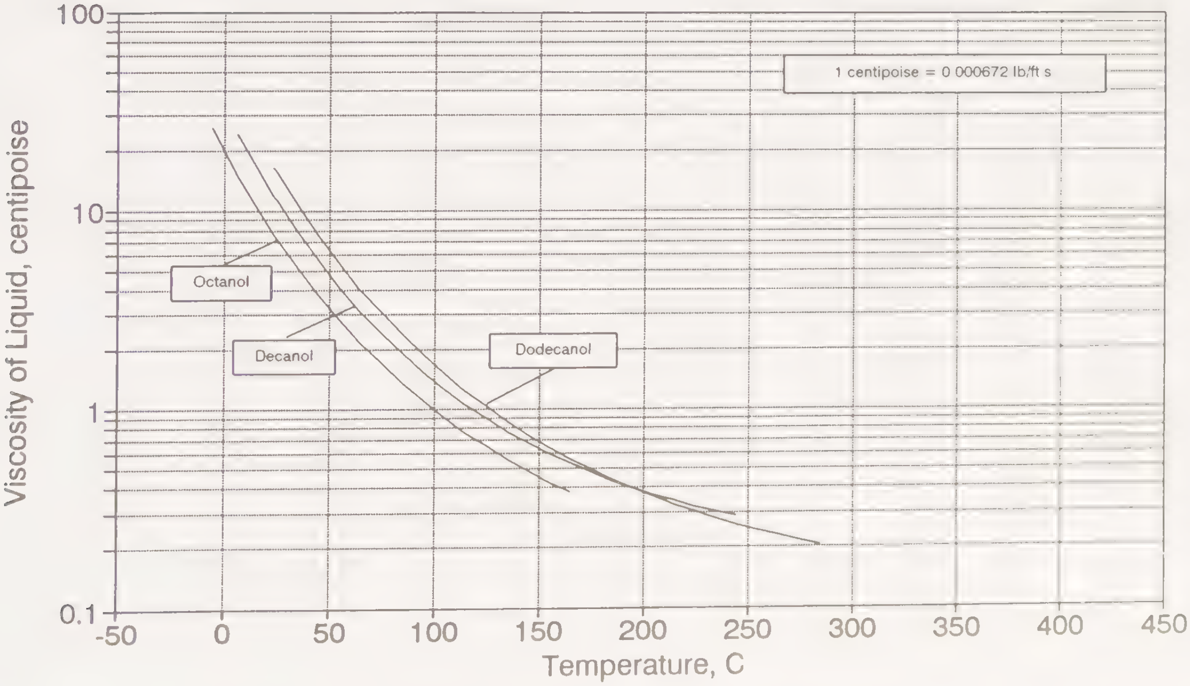

Figure 7-8 Viscosity of Liquid

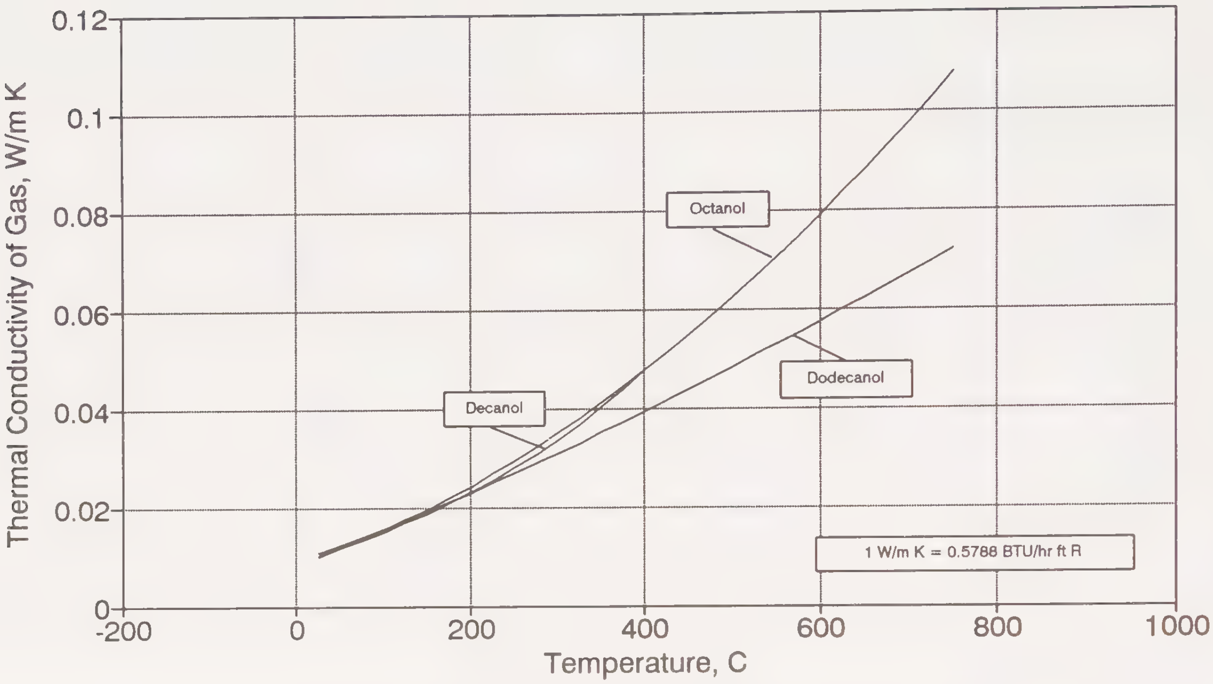

Figure 7-9 Thermal Conductivity of Gas

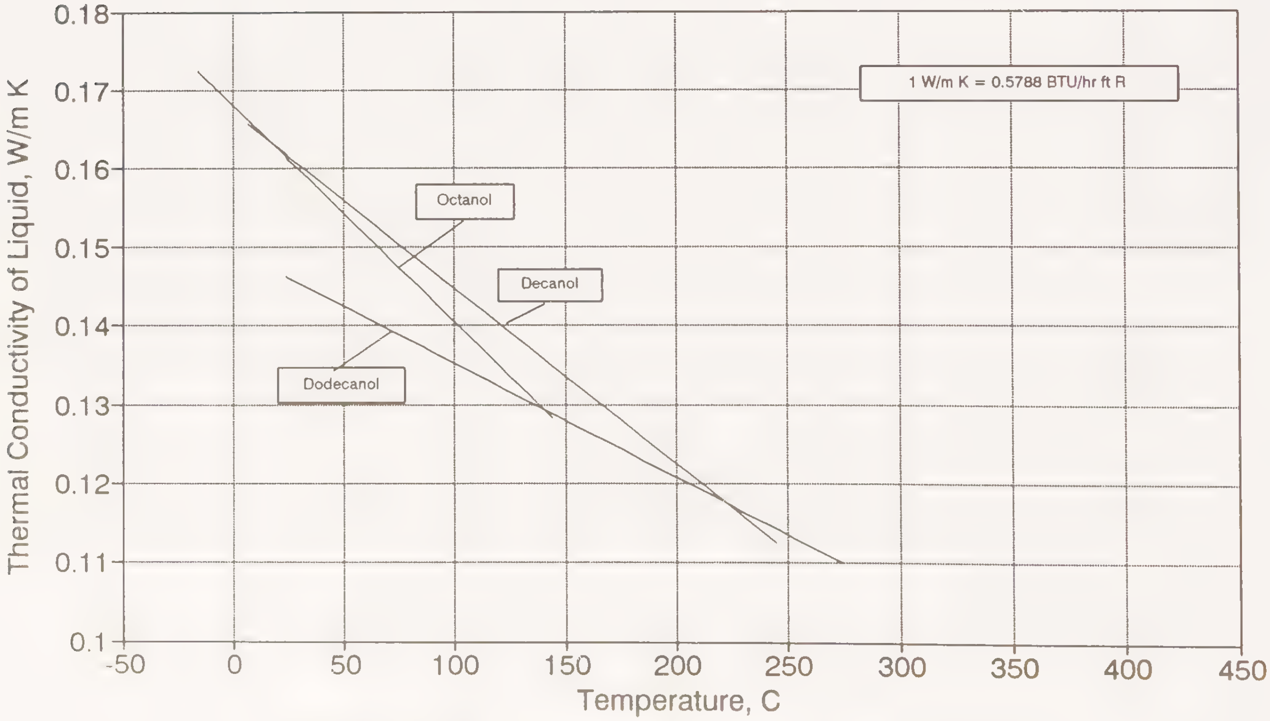

Figure 7-10 Thermal Conductivity of Liquid

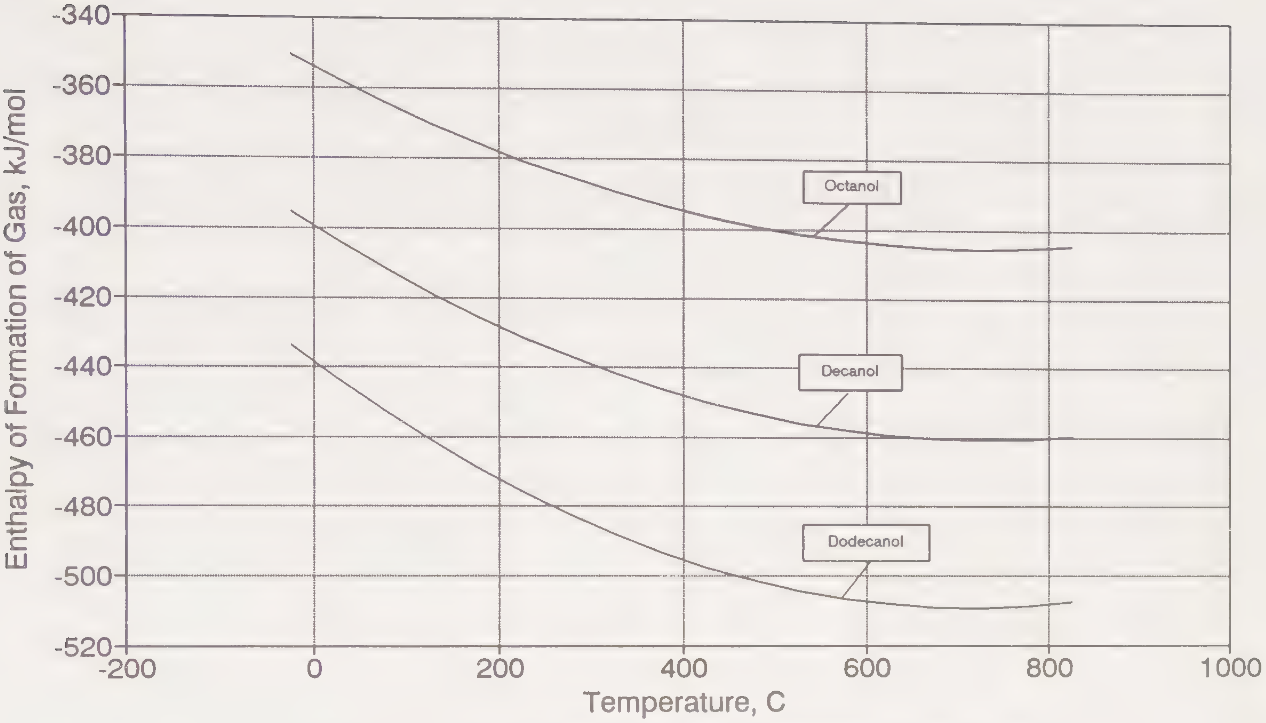

Figure 7-11 Enthalpy of Formation of Gas

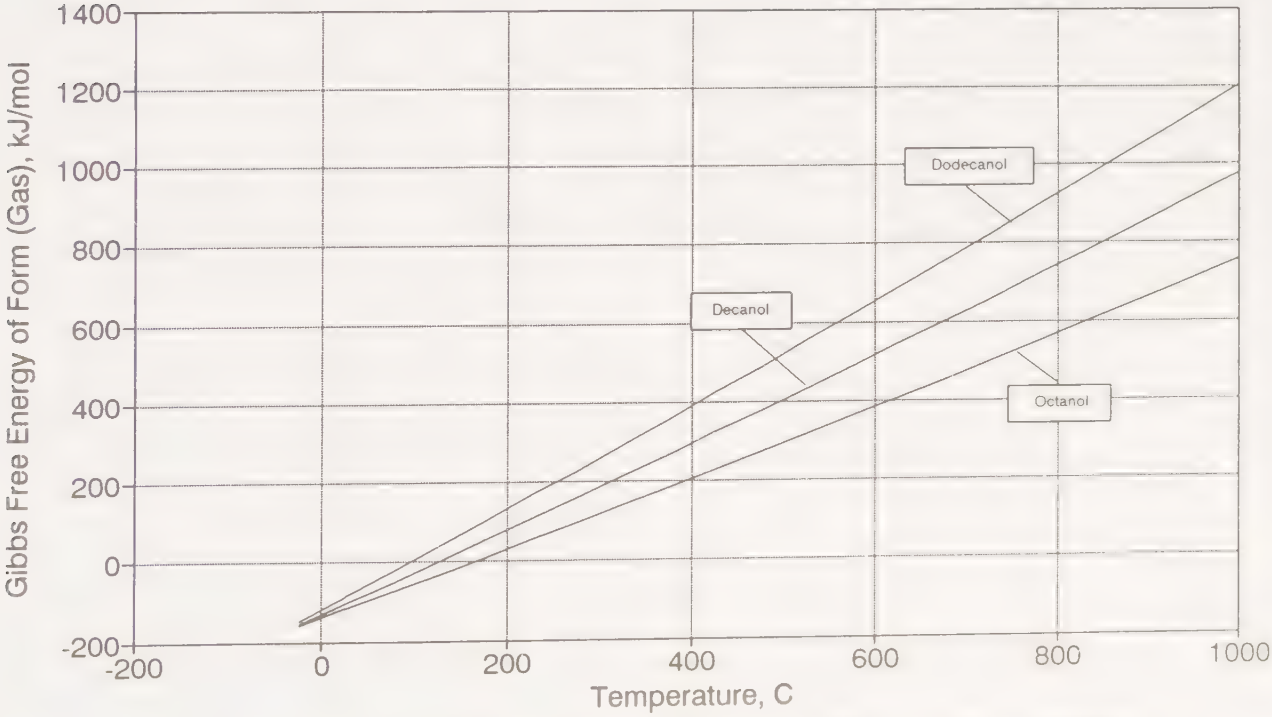

Figure 7-12 Gibbs Free Energy of Formation of Gas

Chapter 8

C_{14}, C_{16} and C_{18} NORMAL ALCOHOL

Robert W. Gallant, Carl L. Yaws and Li Bu

PHYSICAL PROPERTIES - Table 8-1

Property data from the literature (2,3,21,63,65,66,72,89,90,100-103) are given in Table 8-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available. The DIPPR (Design Institute for Physical Property Research) project (5) and data compilations by Yaws and co-workers (44) were consulted extensively in preparing the tabulation.

VAPOR PRESSURE - Figure 8-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 10% or less in most cases.

HEAT OF VAPORIZATION - Figure 8-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 10%.

LIQUID DENSITY - Figure 8-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 1% in most cases.

SURFACE TENSION - Figure 8-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 8-5 and 8-6

Results from Yaws and co-workers (44,54) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5b). Results are in favorable agreement with data. Errors are about 1% or less in most cases.

Results from Yaws and co-workers (44,54) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6a). Results are in fair agreement with data. Errors are about 10% or less in most cases.

VISCOSITY - Figures 8-7 and 8-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 0% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 10% or less in most cases.

THERMAL CONDUCTIVITY - Figures 8-9 and 8-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is fair with possible errors of 10%.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most case.

ENTHALPY OF FORMATION - Figure 8-11

The data compilation of Yaws and co-workers (44,45) was selected for enthalpy of formation of ideal gas. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 8-12

The data compilation of Yaws and co-workers (44) was selected for Gibb's free energy of formation of ideal gas. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 8-1 Physical Properties

1. Name	Tetradecanol	Hexadecanol	Octadecanol
2. Formula	C14H30O	C16H34O	C18H38O
3. Molecular Weight, g/mol	214.392	242.445	270.499
4. Critical Temperature, K	741.00	761.00	777.00
5. Critical Pressure, bar	17.000	15.100	13.600
6. Critical Volume, ml/mol	802.00	907.00	1010.00
7. Critical Compressibility Factor	0.221	0.216	0.213
8. Acentric Factor	0.6765	0.7480	0.8634
9. Melting Point, K	310.65	322.35	331.05
10. Boiling Point @ 1 atm, K	560.15	585.15	608.15
11. Heat of Vaporization @ BP, kJ/kg	262.03	243.66	229.83
12. Density of Liquid @ BP, g/ml	0.628	0.614	0.600
13. Surface Tension @ BP, dynes/cm	9.649	9.088	8.306
14. Heat Capacity of Gas @ 25 C, J/g K	1.579	1.585	2.005
15. Heat Capacity of Liquid @ BP, J/g K	1.988	2.419	2.150
16. Viscosity of Gas @ 25 C, micropoise	44.012	41.290	39.179
17. Viscosity of Liquid @ BP, centipoise	0.075	0.046	0.052
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.007	0.008	0.009
19. Thermal Conductivity of Liquid @ BP, W/m K	0.120	0.085	0.112
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-484.47	-525.69	-566.96
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-70.91	-54.17	-37.45
22. Flash Point, K	414.15	428.00	450.00
23. Autoignition Temperture, K	------	------	------
24. Lower Explosion Limit in Air, vol %	0.5	0.5	0.4
25. Upper Explosion Limit in Air, vol %	------	------	------
26. Solubility in Water @ 25 C, ppm(wt)	0.3000	0.0350	0.0011 @ 34 C

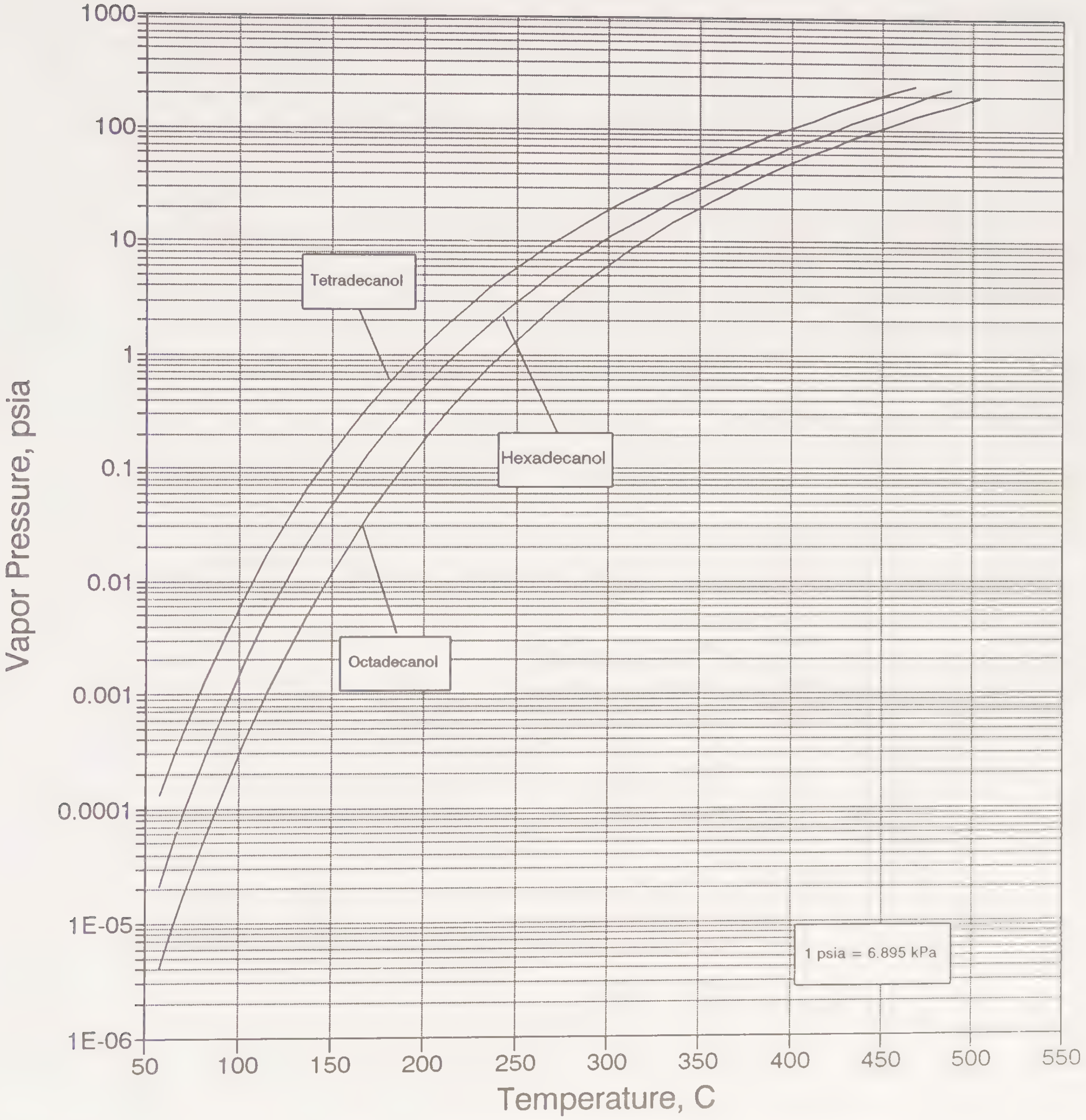

Figure 8-1 Vapor Pressure

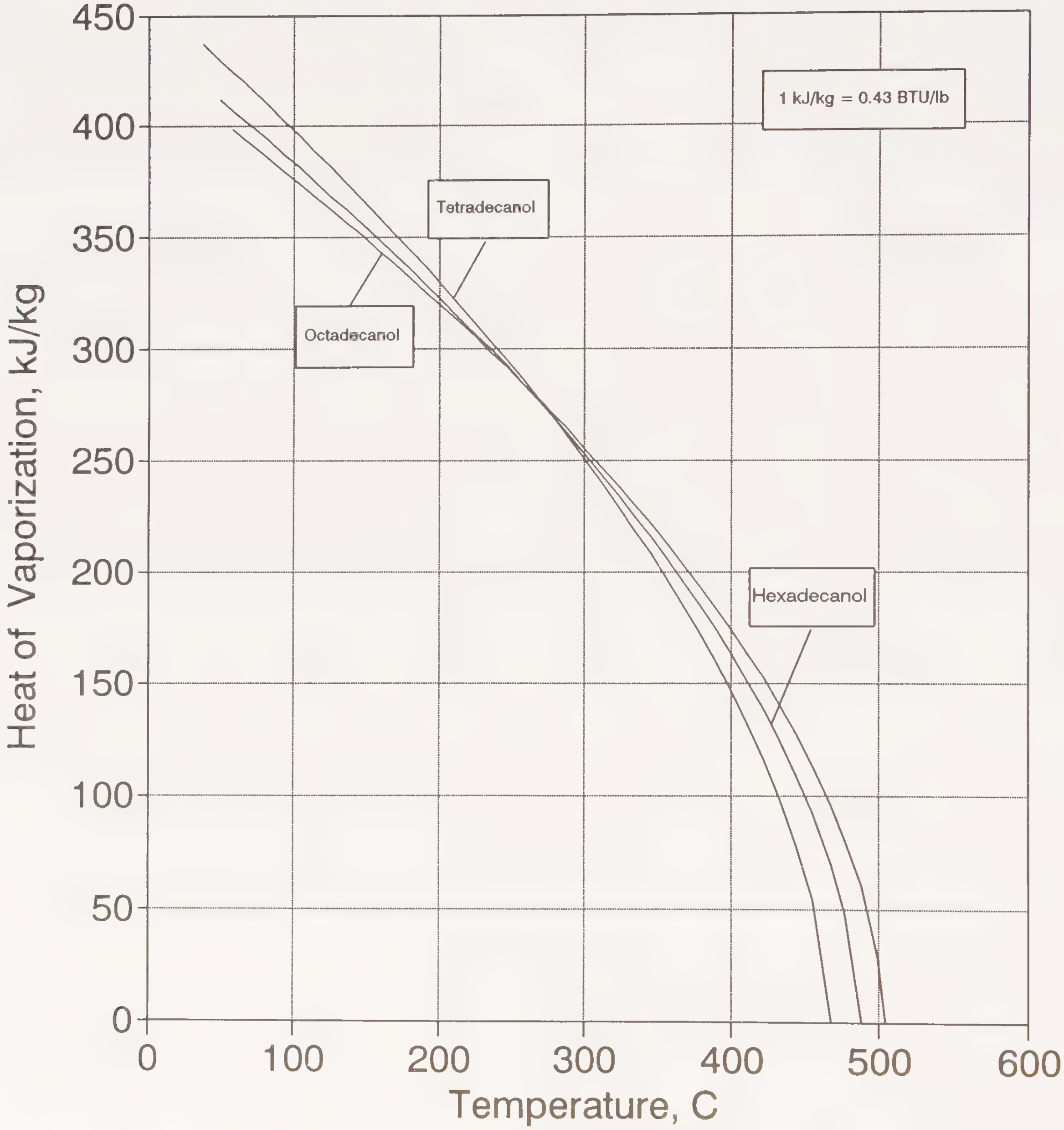

Figure 8-2 Heat of Vaporization

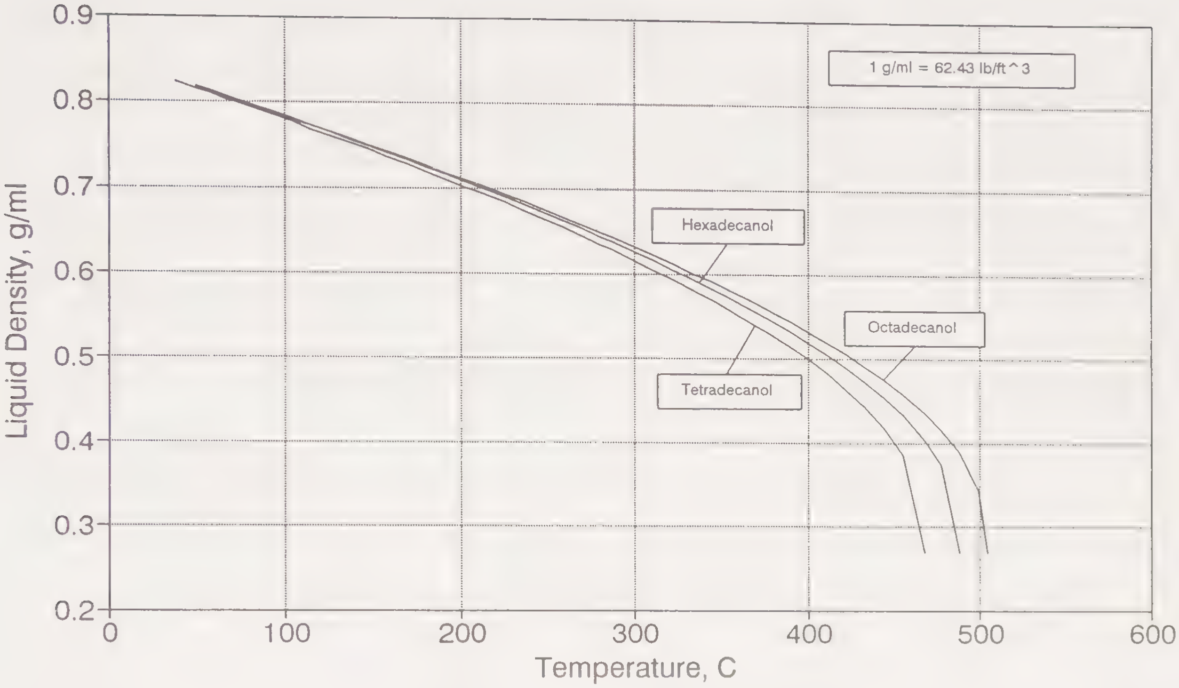

Figure 8-3 Liquid Density

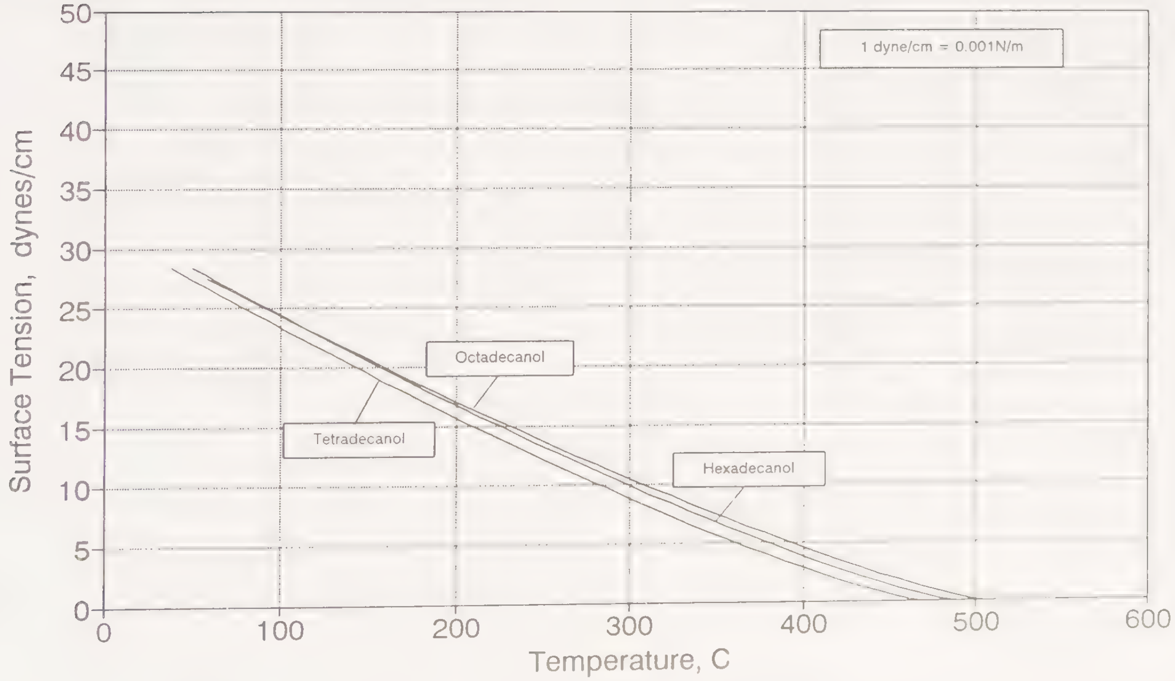

Figure 8-4 Surface Tension

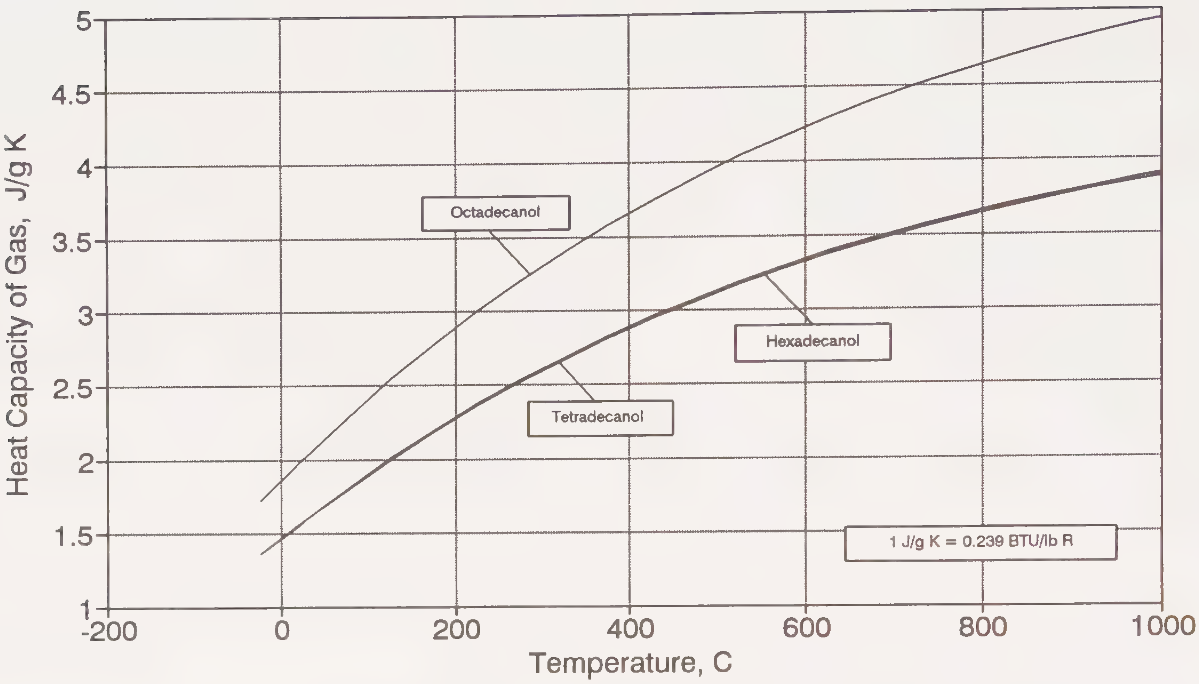

Figure 8-5 Heat Capacity of Gas

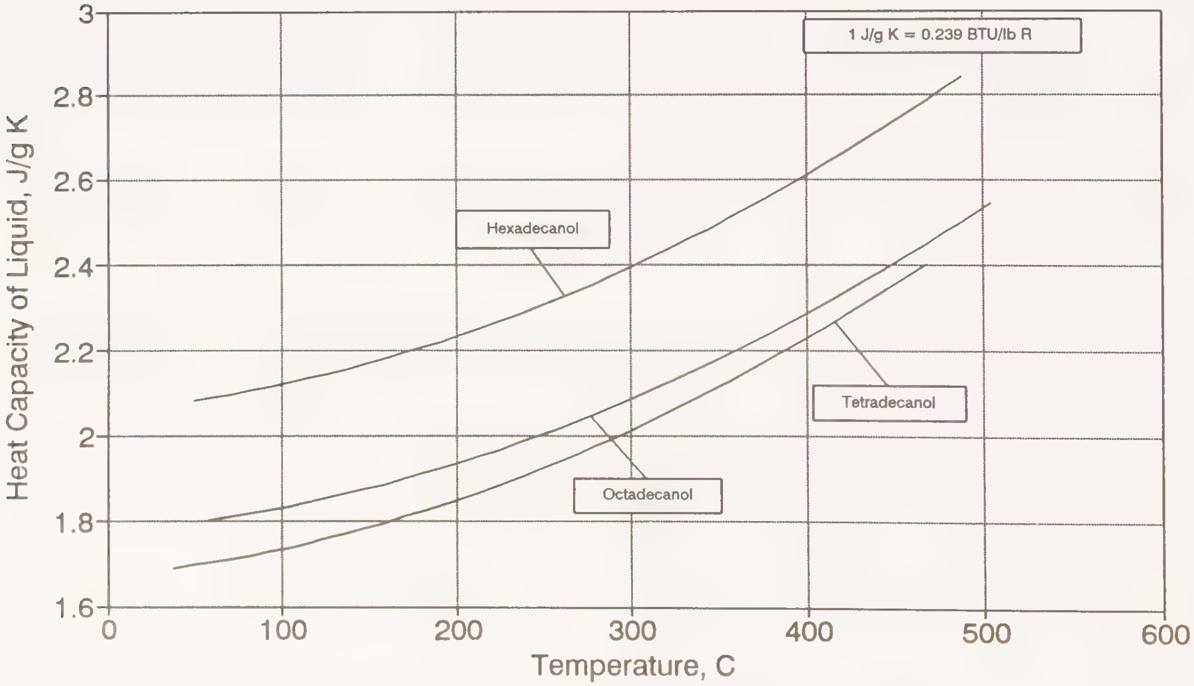

Figure 8-6 Heat Capacity of Liquid

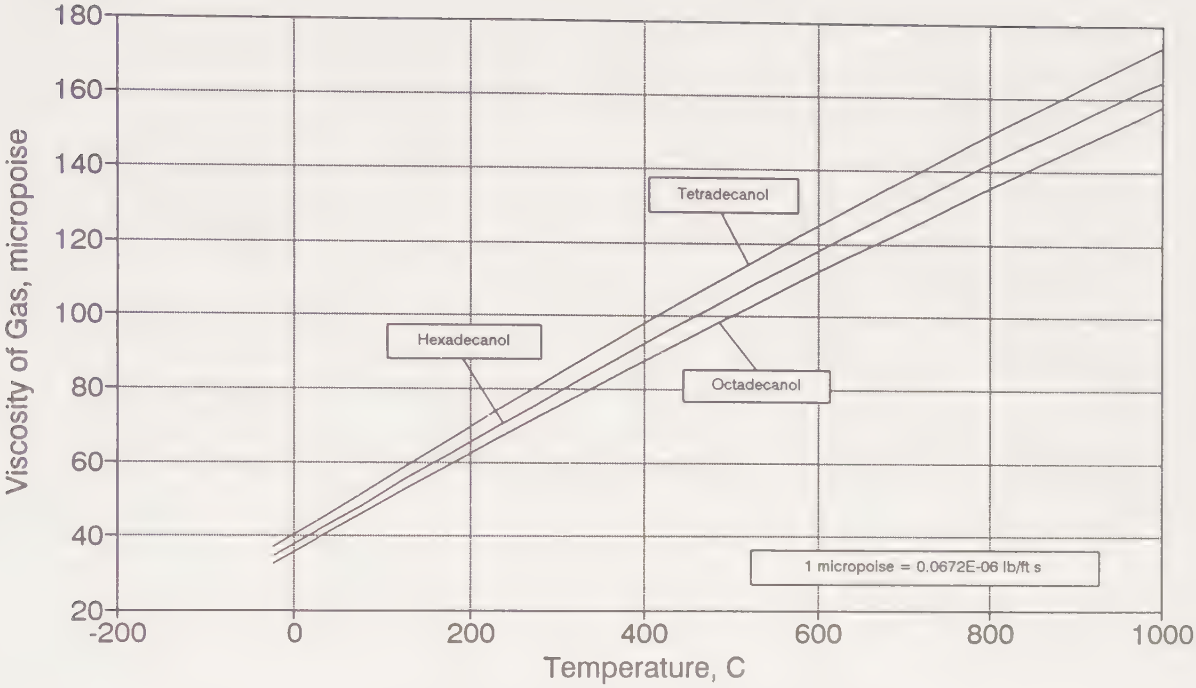

Figure 8-7 Viscosity of Gas

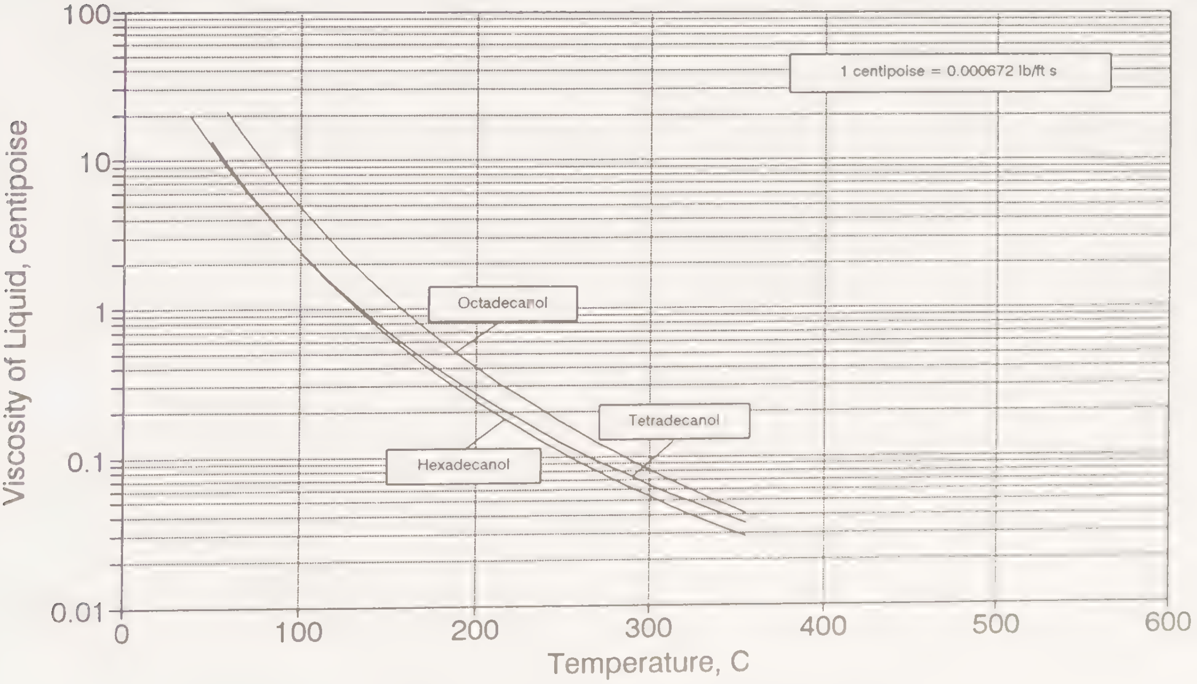

Figure 8-8 Viscosity of Liquid

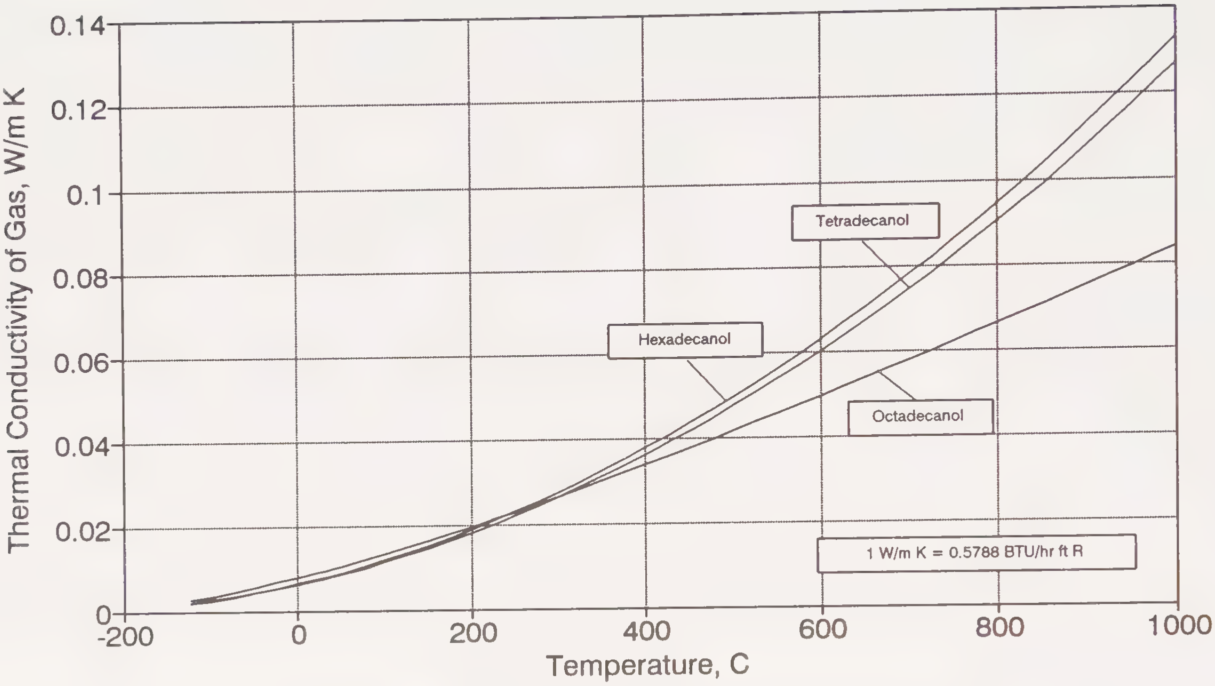

Figure 8-9 Thermal Conductivity of Gas

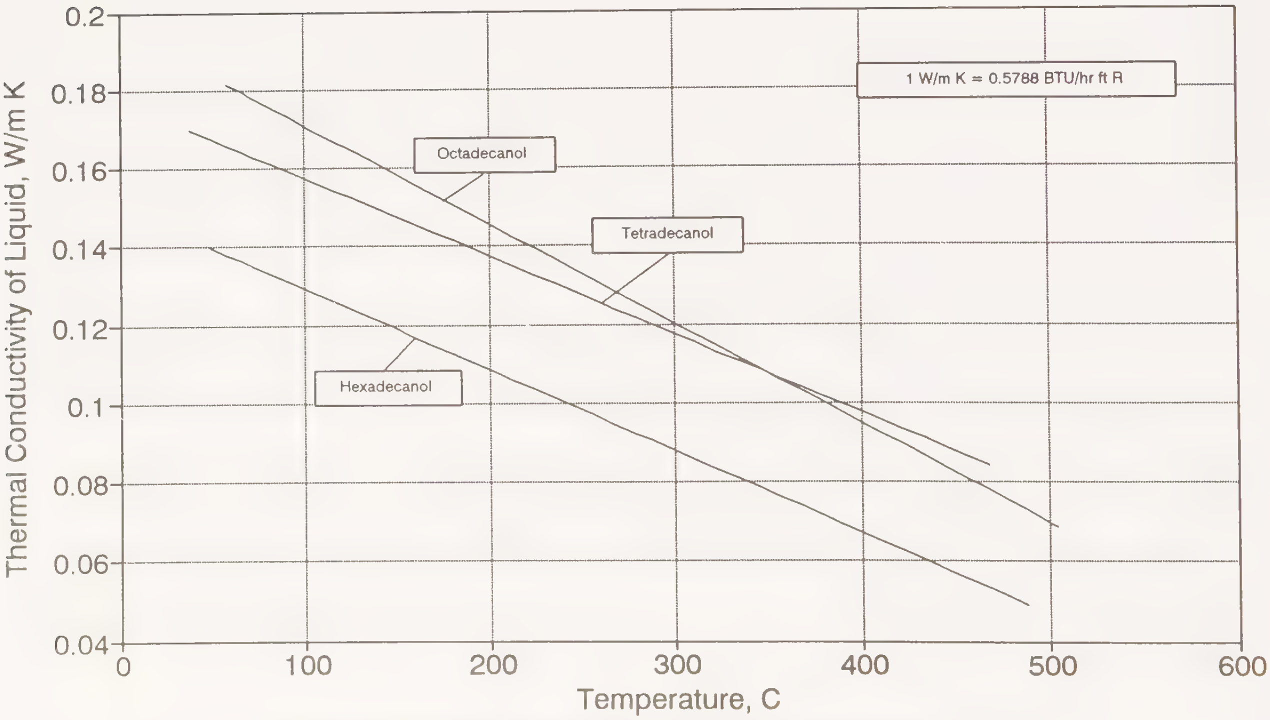

Figure 8-10 Thermal Conductivity of Liquid

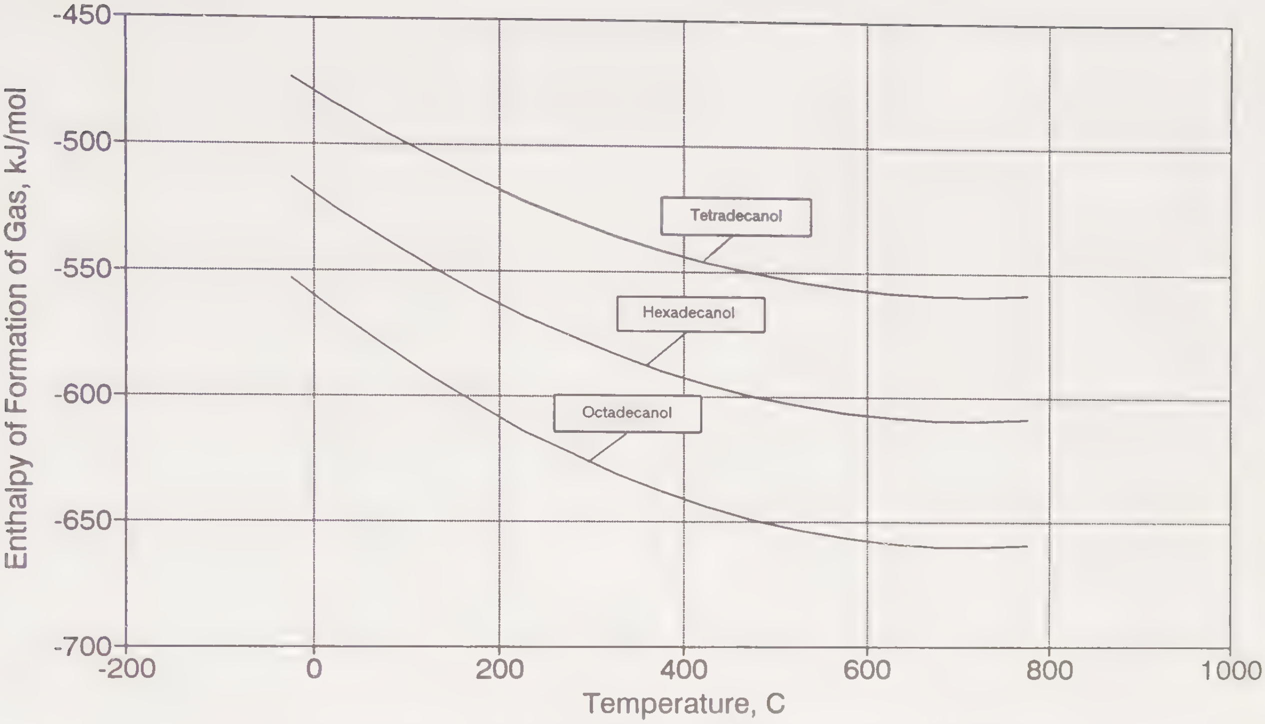

Figure 8-11 Enthalpy of Formation of Gas

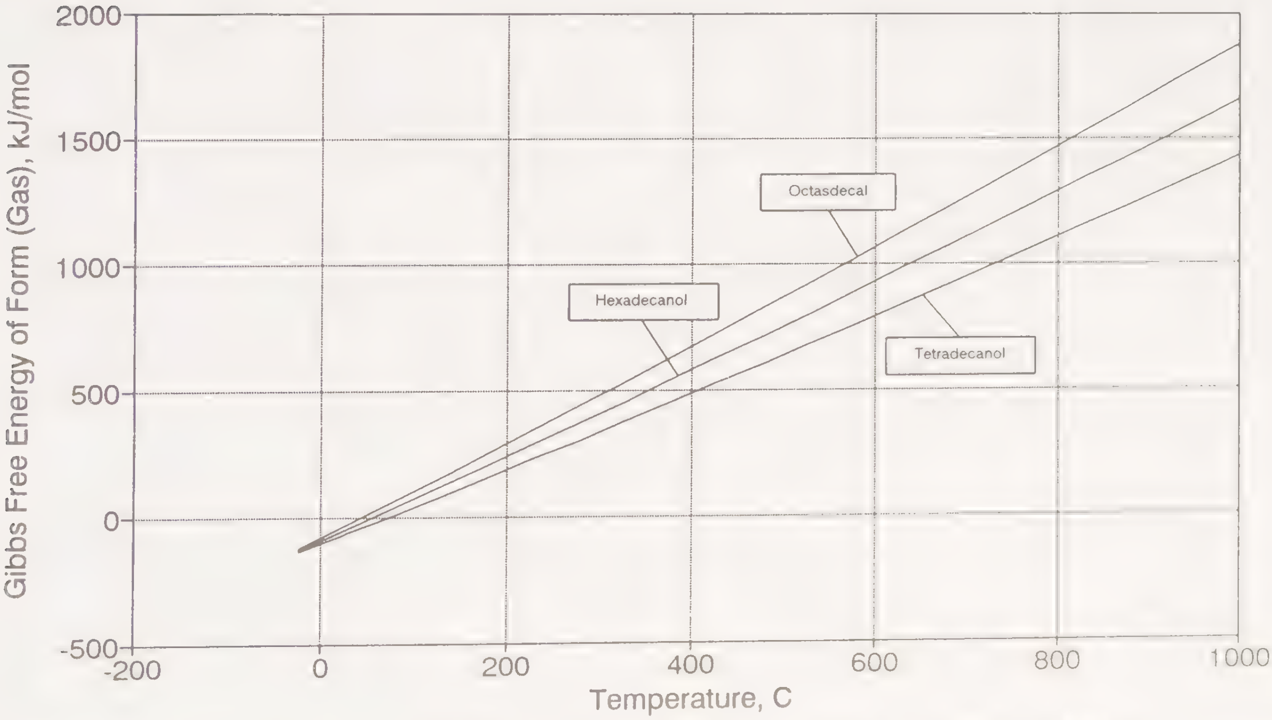

Figure 8-12 Gibbs Free Energy of Formation of Gas

Chapter 9

C_5 KETONES

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 9-1

Property data from the literature (2,3,8,21-26,33-36,63-66,73-77,80,89-90,109,155,162-166) are given in Table 9-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 9-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 9-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 5%.

LIQUID DENSITY - Figure 9-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 5% in most cases.

SURFACE TENSION - Figure 9-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 9-5 and 9-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 3% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 3% or less in most cases. The liquid heat capacity of methyl propyl ketone was assumed to approximately equal to that of diethyl ketone.

VISCOSITY - Figures 9-7 and 9-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 3% or less in most cases except for methyl isopropyl ketone (possible 10% error).

THERMAL CONDUCTIVITY - Figures 9-9 and 9-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is fair with errors less then 10% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 9-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 9-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 9-1 Physical Properties

1. Name	Methyl Isopropyl Ketone	Diethyl Ketone	Methyl Propyl Ketone
2. Formula	C5H10O	C5H10O	C5H10O
3. Molecular Weight, g/mol	86.134	86.134	86.134
4. Critical Temperature, K	553.00	560.95	561.08
5. Critical Pressure, bar	38.504	37.389	36.943
6. Critical Volume, ml/mol	310.00	336.00	301.00
7. Critical Compressibility Factor	0.260	0.269	0.238
8. Acentric Factor	0.3500	0.3502	0.3456
9. Melting Point, K	181.15	234.18	196.29
10. Boiling Point @ 1 atm, K	367.55	375.14	375.46
11. Heat of Vaporization @ BP, kJ/kg	391.50	389.75	397.80
12. Density of Liquid @ BP, g/ml	0.805	0.810	0.783
13. Surface Tension @ BP, dynes/cm	24.828	24.561	23.260
14. Heat Capacity of Gas @ 25 C, J/g K	1.302	1.506	1.453
15. Heat Capacity of Liquid @ BP, J/g K	2.089	2.215	2.215
16. Viscosity of Gas @ 25 C, micropoise	66.165	65.471	64.160
17. Viscosity of Liquid @ BP, centipoise	0.430	0.443	0.471
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.012	0.011	0.011
19. Thermal Conductivity of Liquid @ BP, W/m K	0.143	0.143	0.142
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-263.15	-258.70	-259.62
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-140.31	-136.18	-139.57
22. Flash Point, K	273.00	285.93	280.37
23. Autoignition Temperture, K	------	725.37	725.15
24. Lower Explosion Limit in Air, vol %	1.5	1.5	1.5
25. Upper Explosion Limit in Air, vol %	9.0	8.0	8.2
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

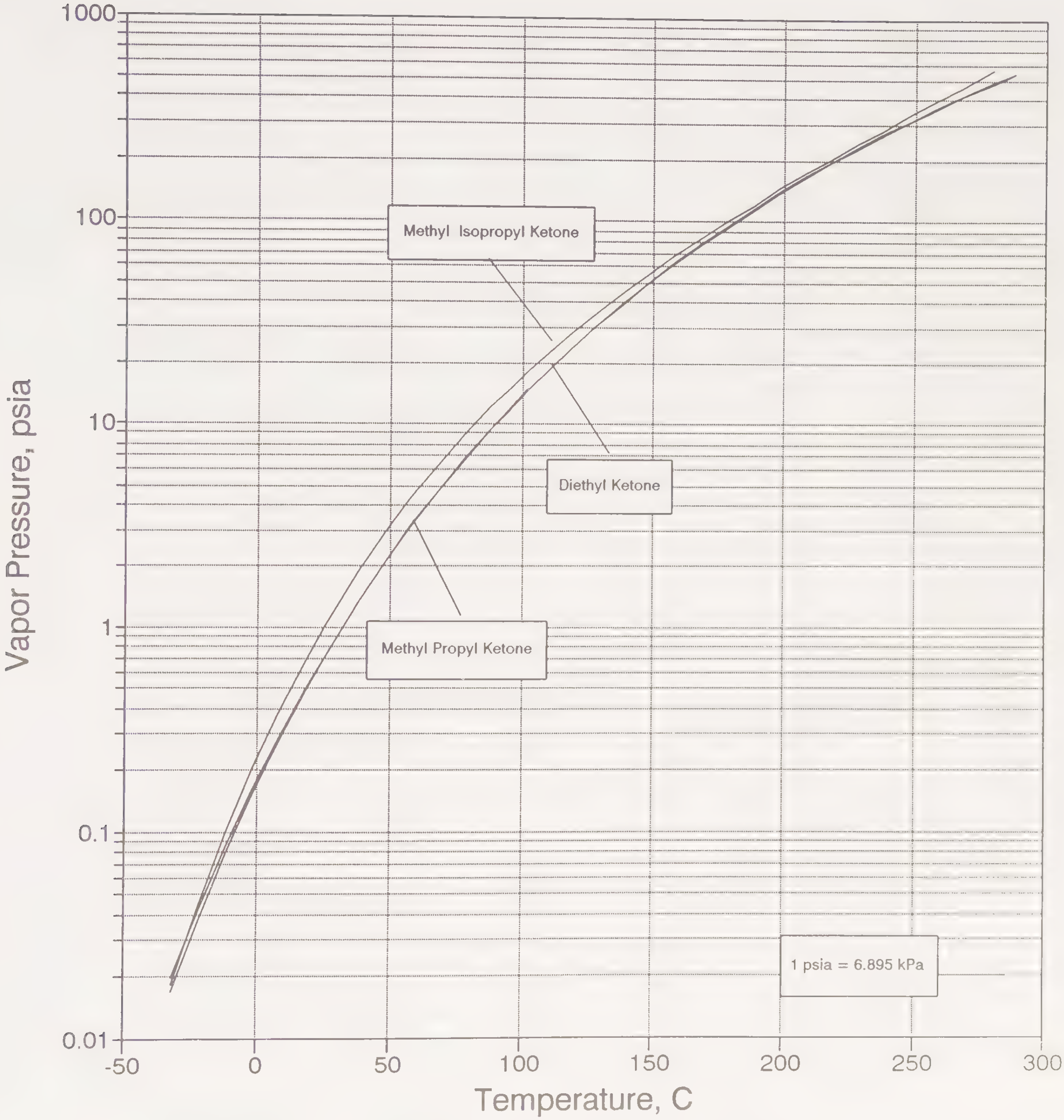

Figure 9-1 Vapor Pressure

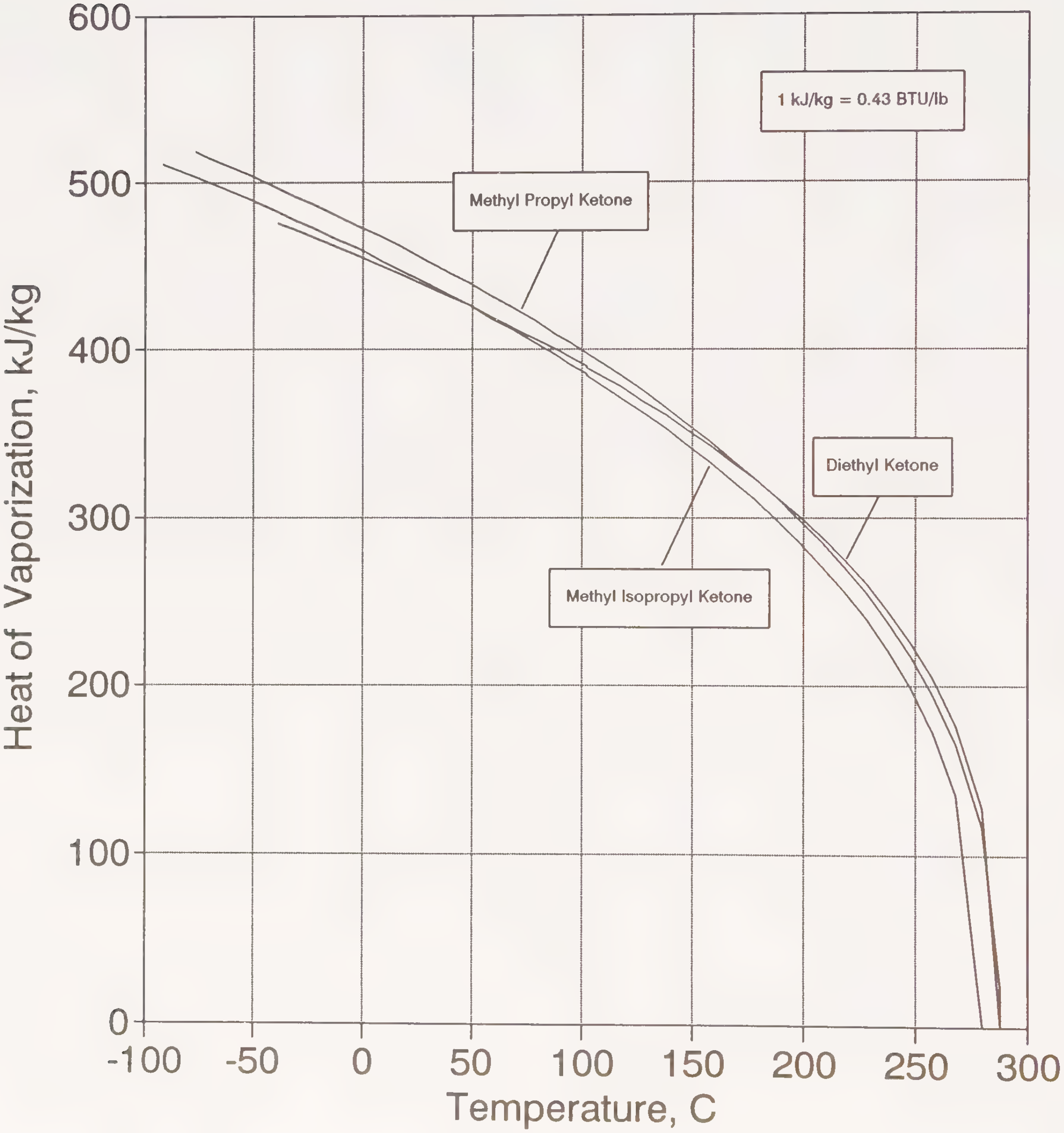

Figure 9-2 Heat of Vaporization

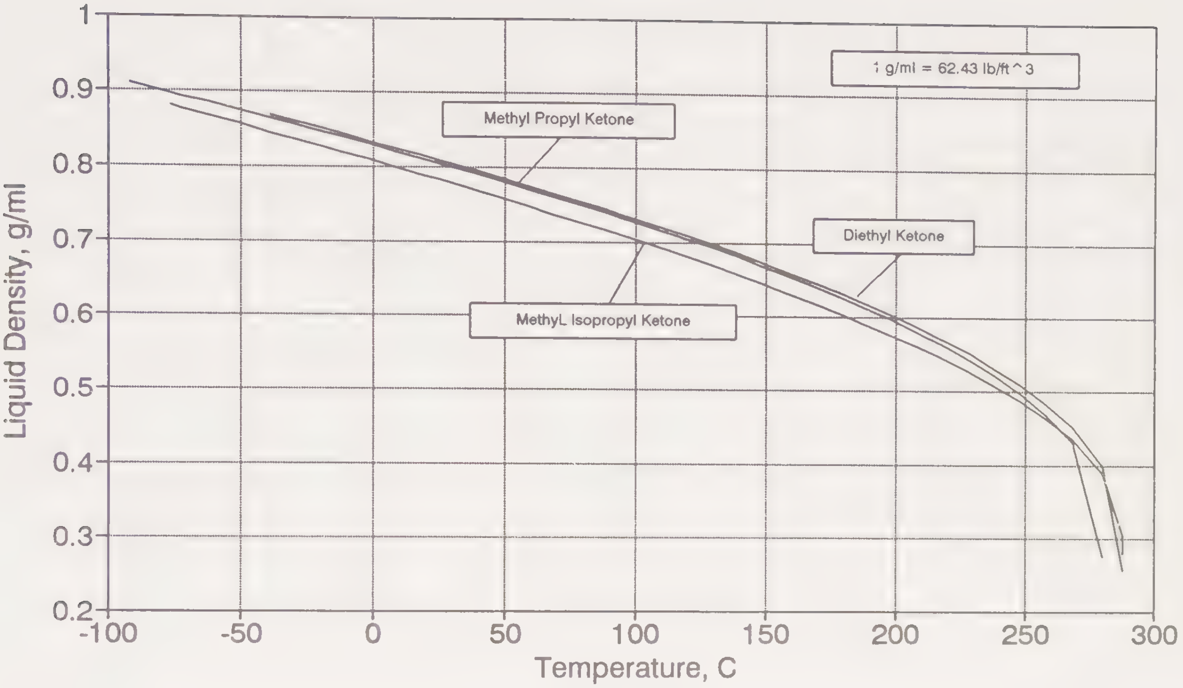

Figure 9-3 Liquid Density

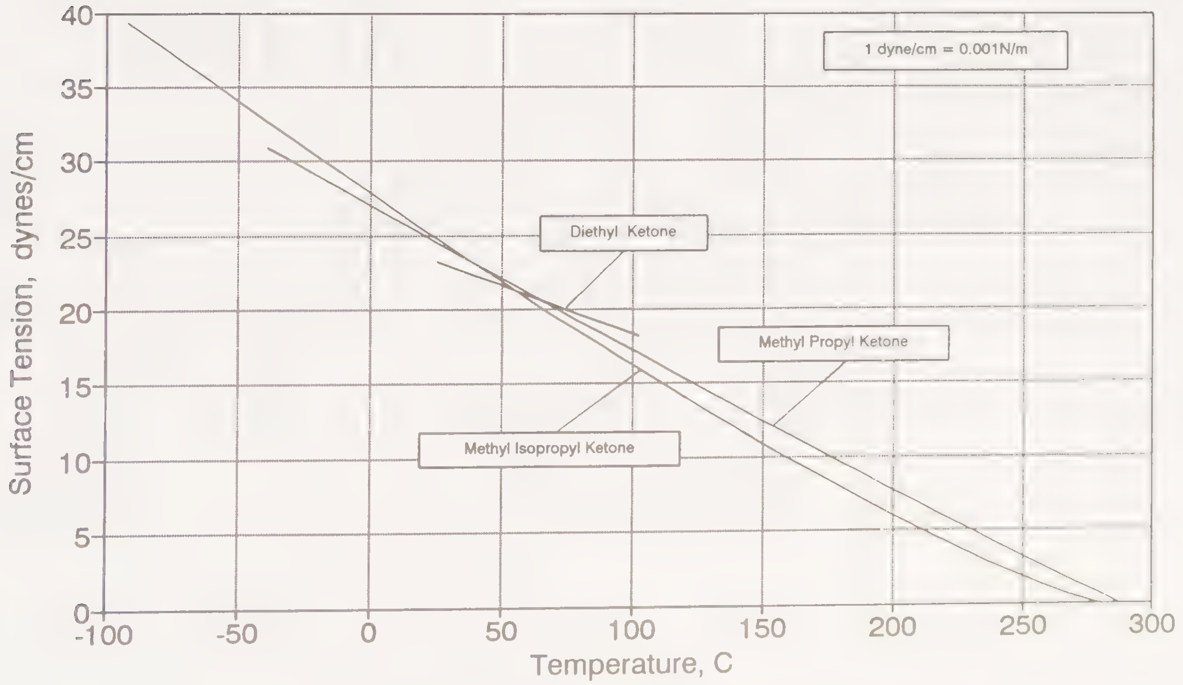

Figure 9-4 Surface Tension

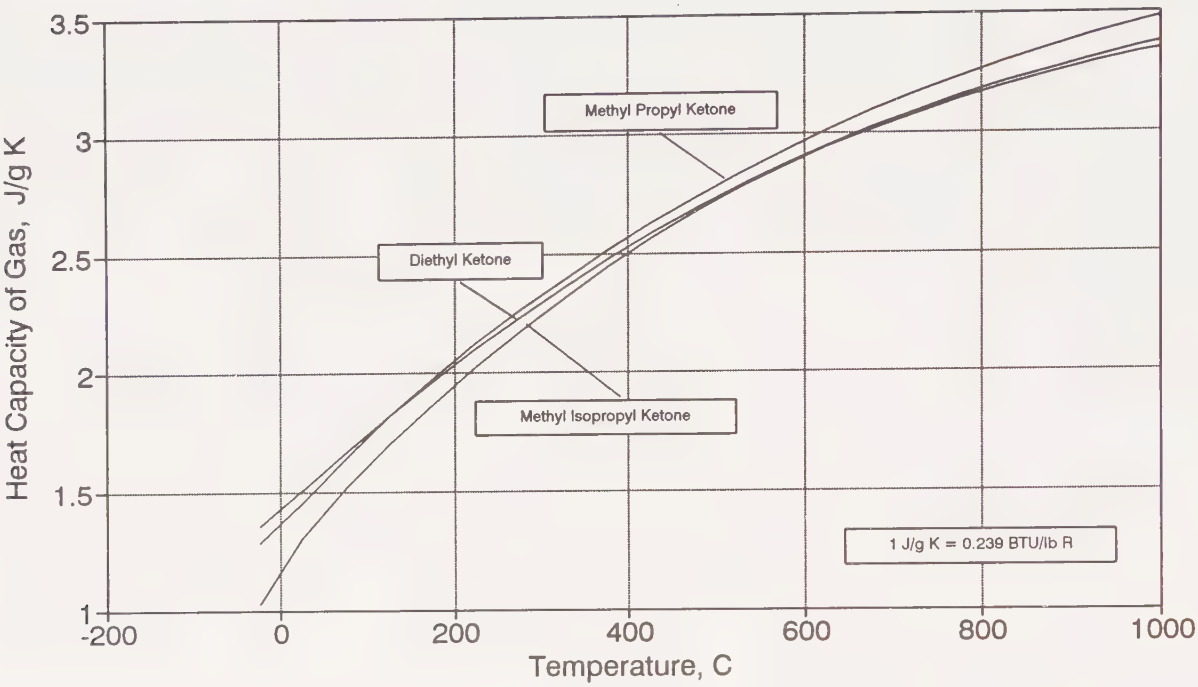

Figure 9-5 Heat Capacity of Gas

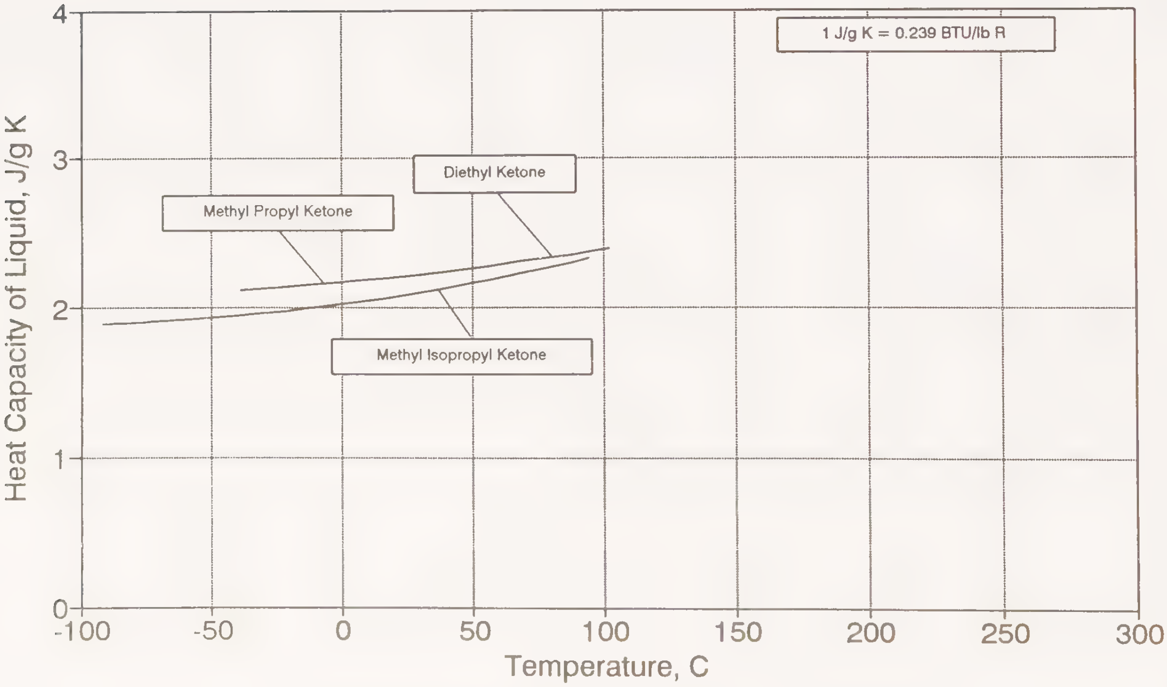

Figure 9-6 Heat Capacity of Liquid

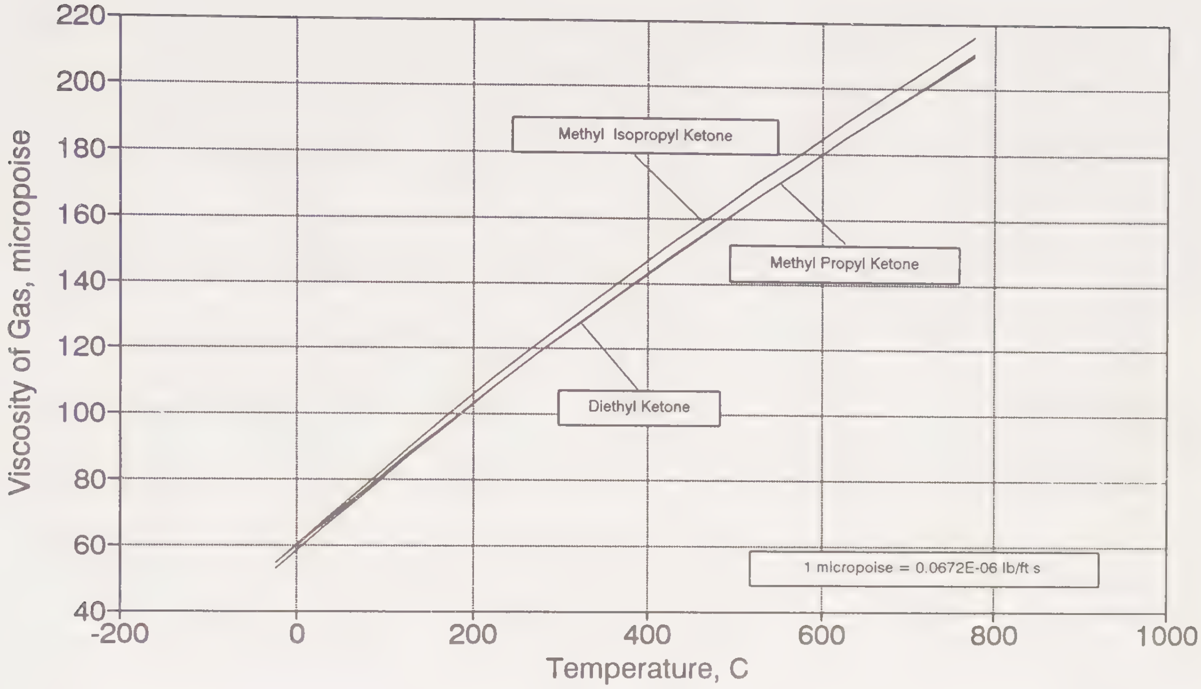

Figure 9-7 Viscosity of Gas

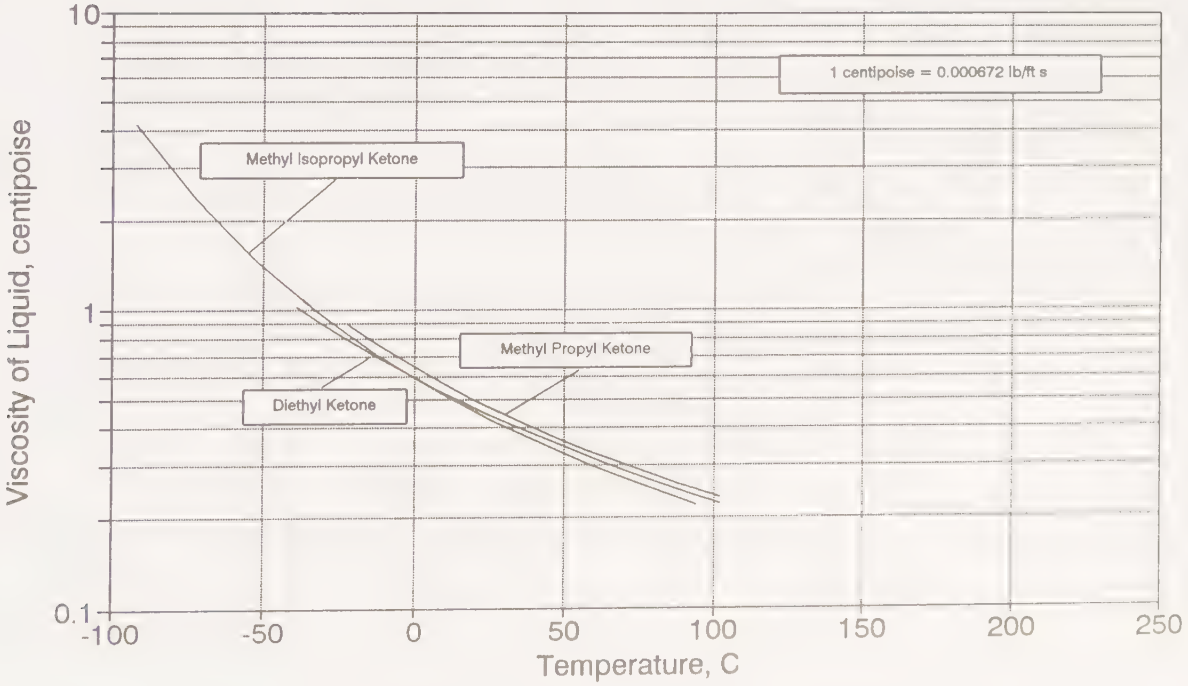

Figure 9-8 Viscosity of Liquid

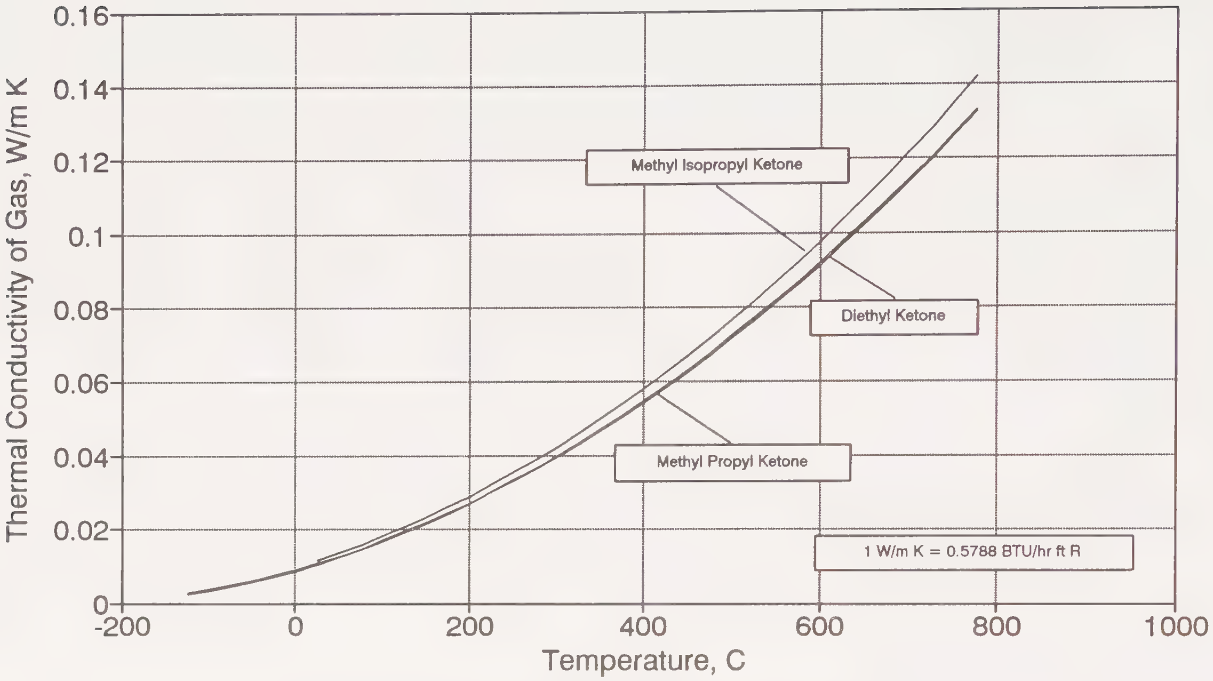

Figure 9-9 Thermal Conductivity of Gas

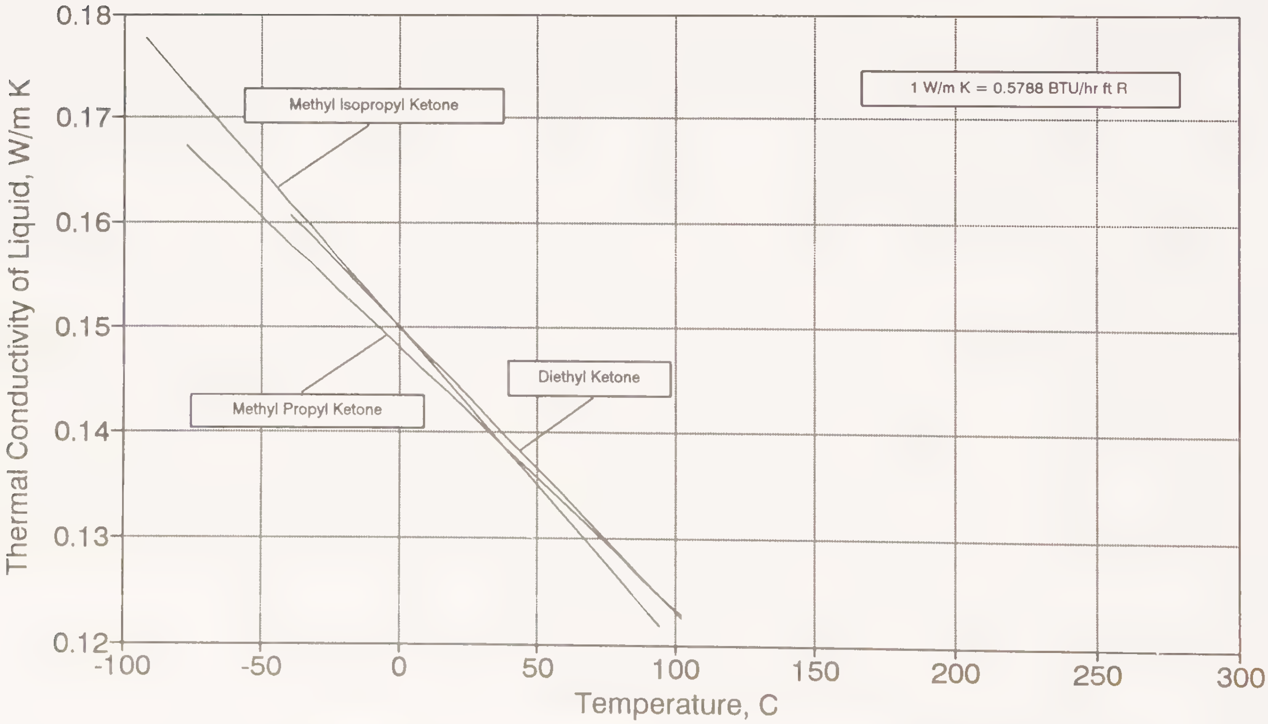

Figure 9-10 Thermal Conductivity of Liquid

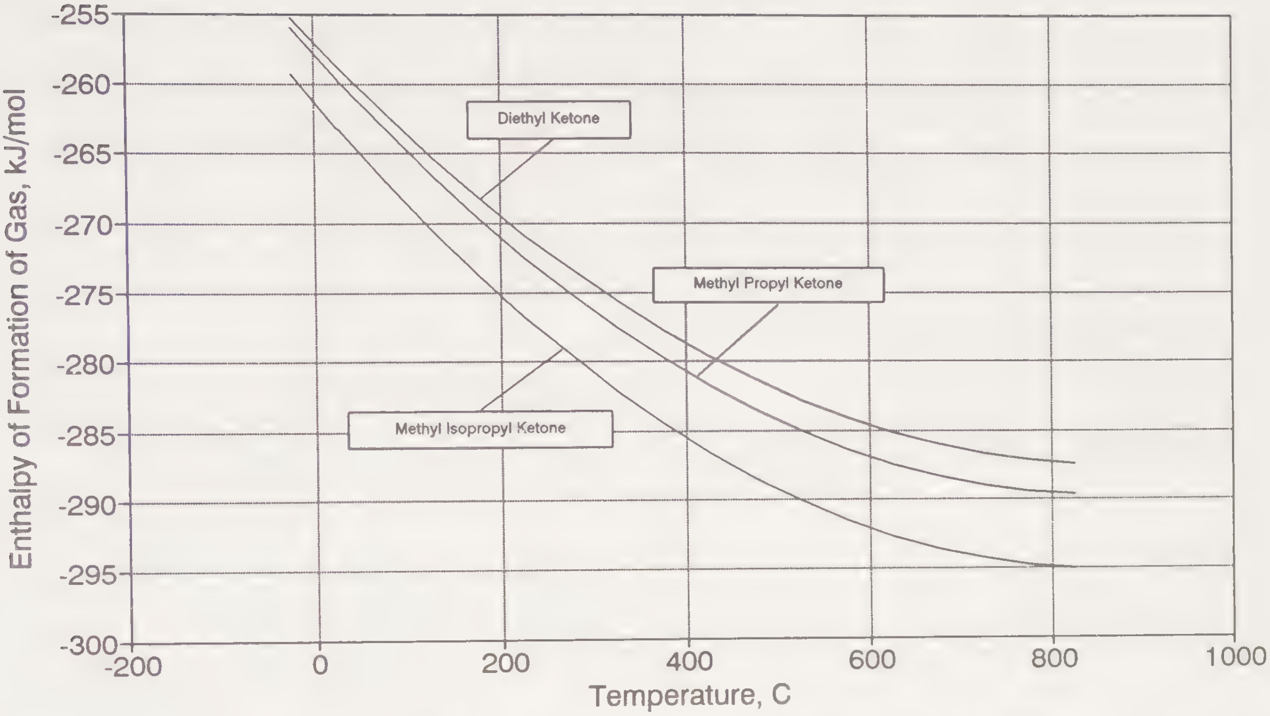

Figure 9-11 Enthalpy of Formation of Gas

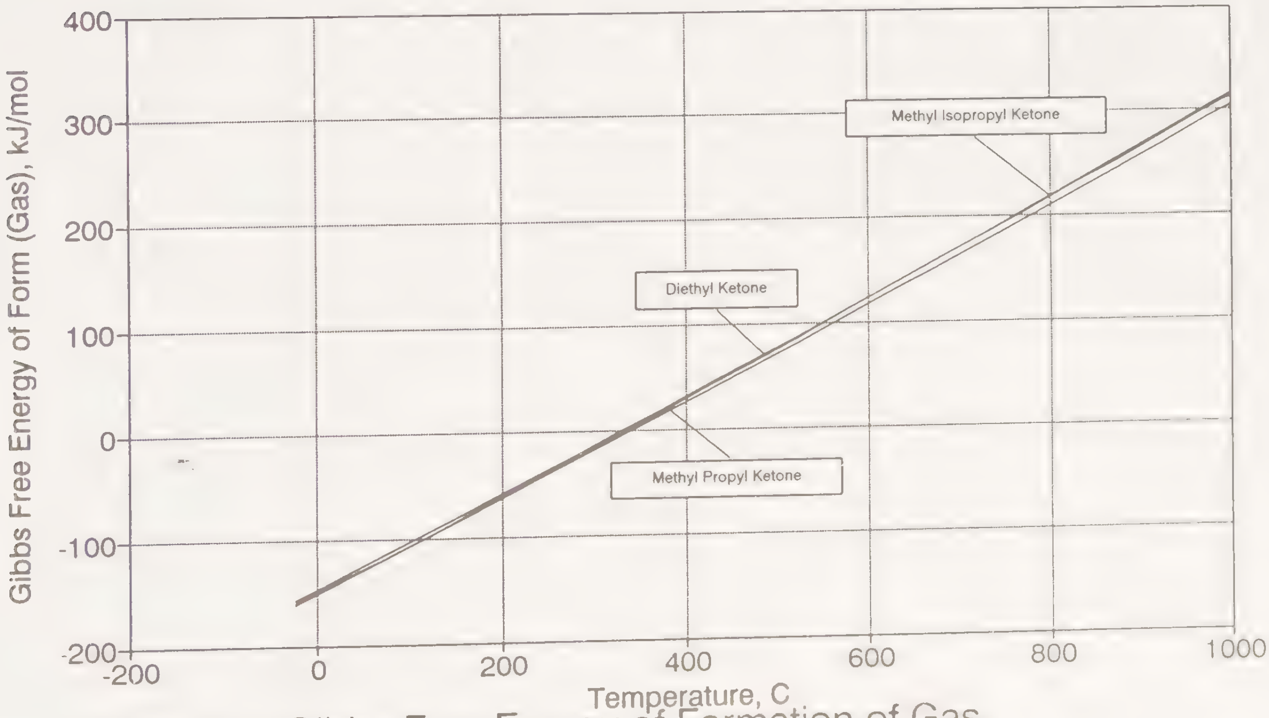

Figure 9-12 Gibbs Free Energy of Formation of Gas

Chapter 10

C_6 KETONES

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 10-1

Property data from the literature (2,3,8,21-26,30,36,63-68,73-75,82,90,101,155,162-165,176-178) are given in Table 10-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 10-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in fair agreement with experimental data. Errors are about 10% or less in most cases.

HEAT OF VAPORIZATION - Figure 10-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is fair with errors of about 10%.

LIQUID DENSITY - Figure 10-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 5% in most cases.

SURFACE TENSION - Figure 10-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 10-5 and 10-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in fair agreement with data. Errors are about 10% or less in most cases except for methyl isobutyl ketone (possible 25% error).

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 10% or less in most cases except for methyl isobutyl ketone (possible 25% error).

VISCOSITY - Figures 10-7 and 10-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 10% or less in most cases.

THERMAL CONDUCTIVITY - Figures 10-9 and 10-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is fair with errors less then 10% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 10-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 10-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 10-1 Physical Properties

1. Name	Ethyl Isopropyl Ketone	Methyl Isobutyl Ketone	Ethyl Propyl Ketone	Methyl Butyl Ketone
2. Formula	C6H12O	C6H12O	C6H12O	C6H12O
3. Molecular Weight, g/mol	100.161	100.161	100.161	100.161
4. Critical Temperature, K	567.00	571.40	582.82	587.05
5. Critical Pressure, bar	33.200	32.728	33.200	33.235
6. Critical Volume, ml/mol	369.00	369.00	364.00	369.00
7. Critical Compressibility Factor	0.260	0.254	0.249	0.251
8. Acentric Factor	0.3911	0.3887	0.3764	0.3967
9. Melting Point, K	------	189.15	217.50	217.35
10. Boiling Point @ 1 atm, K	386.55	389.65	396.65	400.85
11. Heat of Vaporization @ BP, kJ/kg	337.89	357.59	352.59	365.65
12. Density of Liquid @ 25 C, g/ml	0.806	0.796	0.810	0.807
13. Surface Tension @ 25 C, dynes/cm	23.64	23.50	24.99	25.28
14. Heat Capacity of Gas @ 25 C, J/g K	1.446	1.473	1.521	1.480
15. Heat Capacity of Liquid @ 25 C, J/g K	2.023	2.130	2.163	2.129
16. Viscosity of Gas @ 25 C, micropoise	63.082	62.202	61.464	------
17. Viscosity of Liquid @ 25 C, centipoise	0.542	0.571	0.578	0.583
18. Thermal Conductivity of Gas @ 25 C, W/m K	------	------	------	0.010
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.142	0.141	0.148	0.139
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-286.55	-289.05	-278.18	-280.53
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-134.46	-136.74	-126.63	-131.43
22. Flash Point, K	289.00	288.71	287.15	298.15
23. Autoignition Temperature, K	------	732.04	------	697.04
24. Lower Explosion Limit in Air, vol %	1.3	1.4	1.0	1.2
25. Upper Explosion Limit in Air, vol %	7.8	7.5	8.0	8.0
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------	------

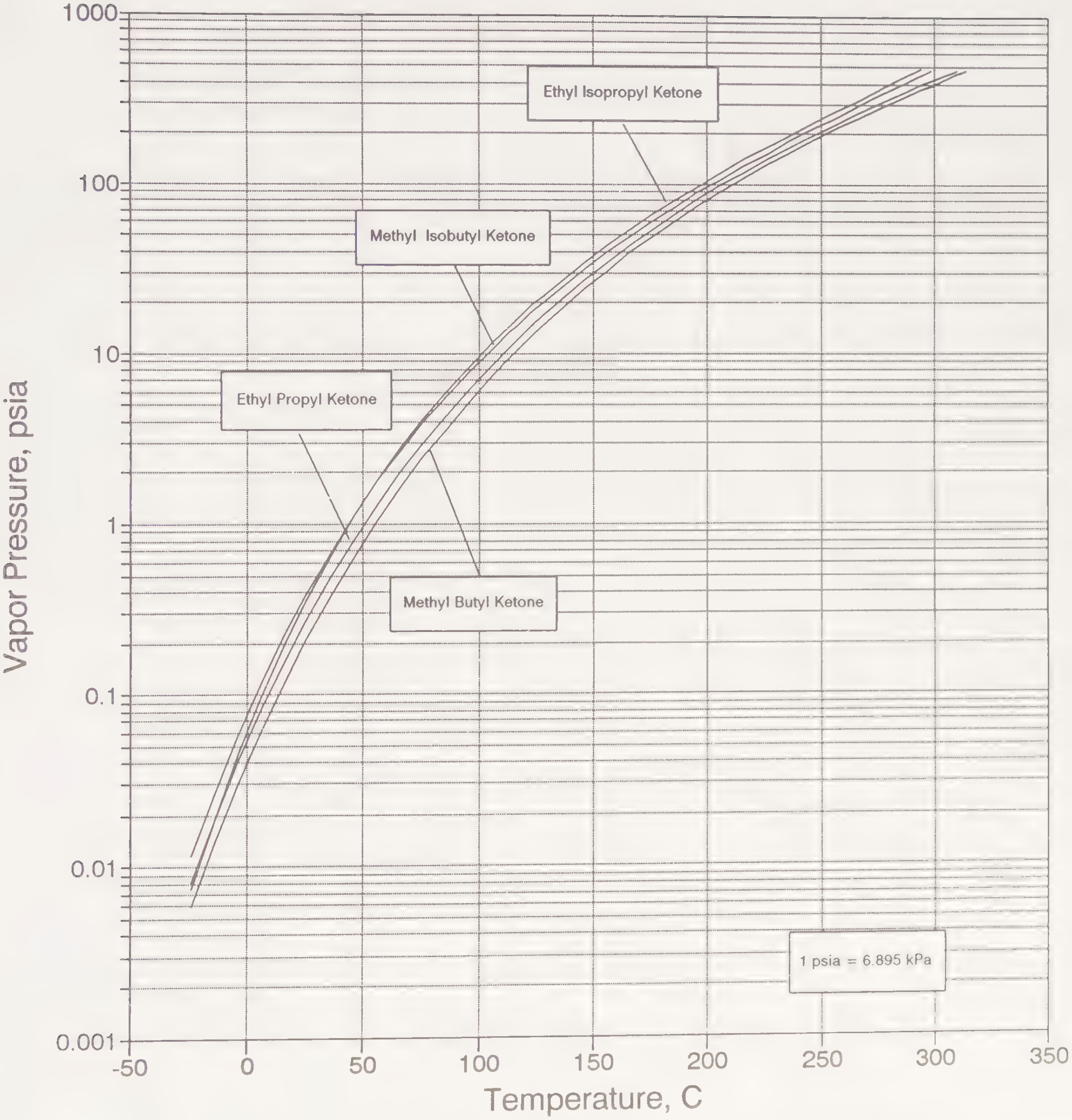

Figure 10-1 Vapor Pressure

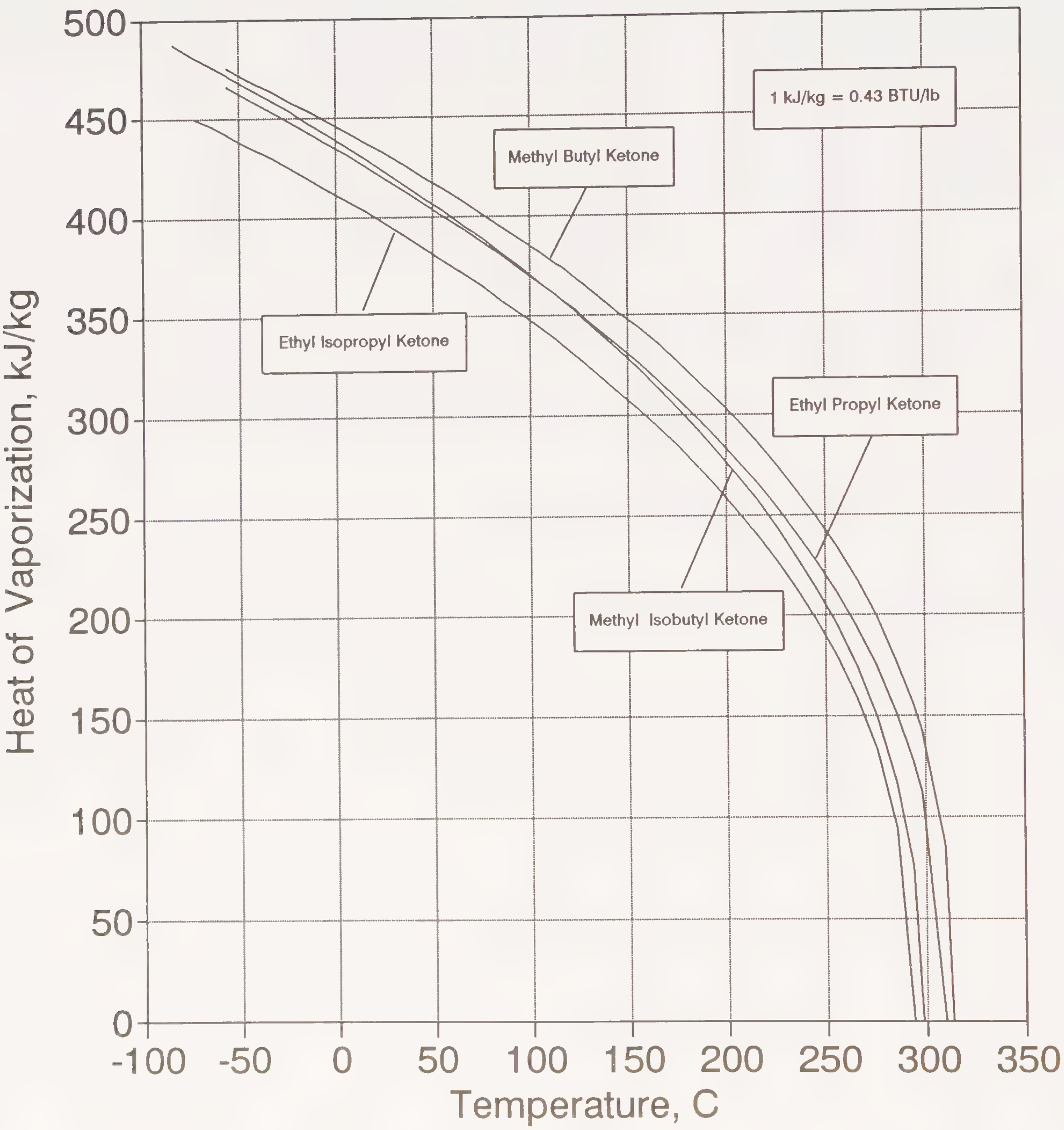

Figure 10-2 Heat of Vaporization

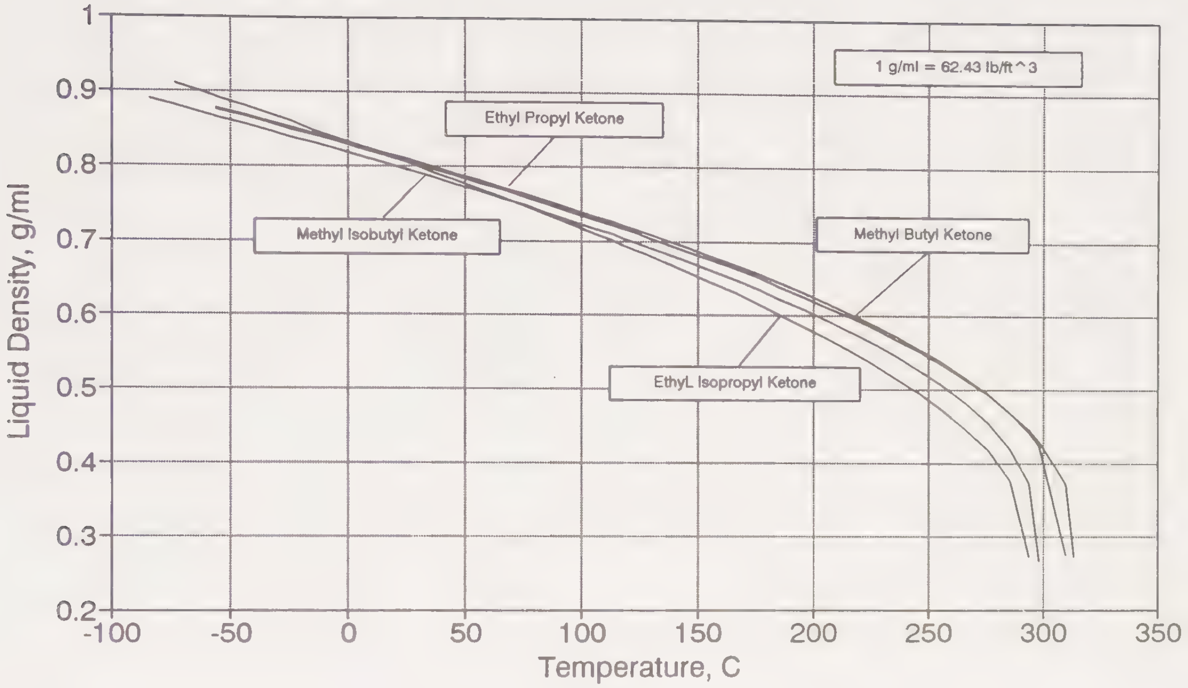

Figure 10-3 Liquid Density

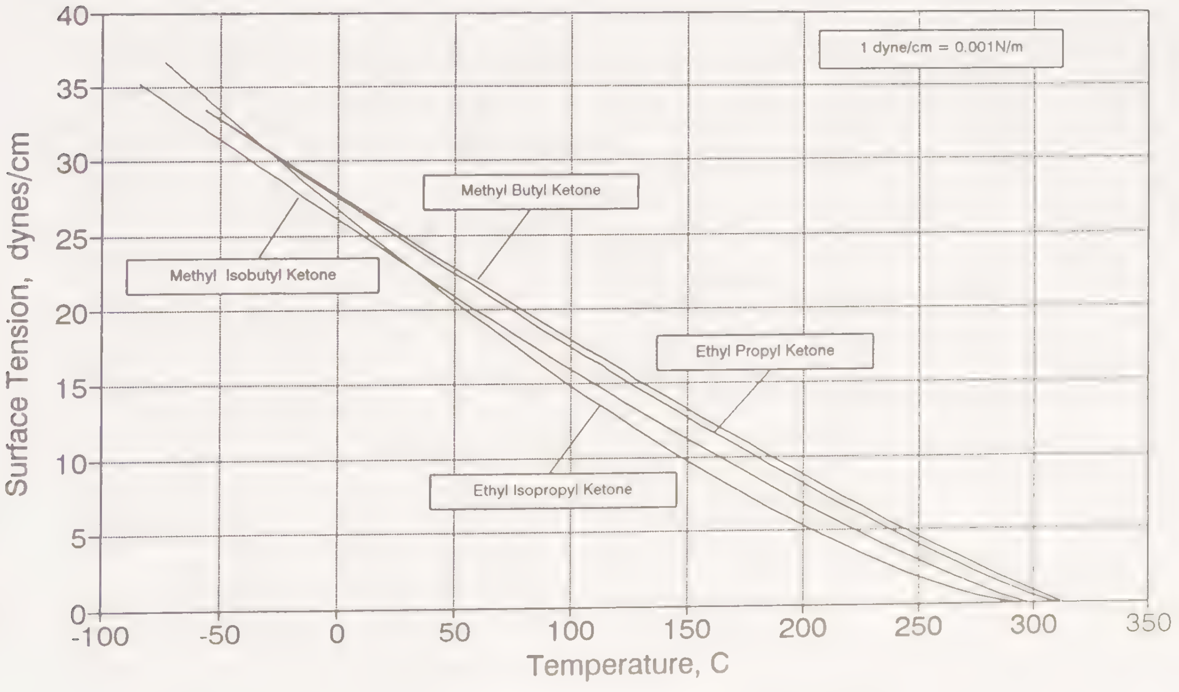

Figure 10-4 Surface Tension

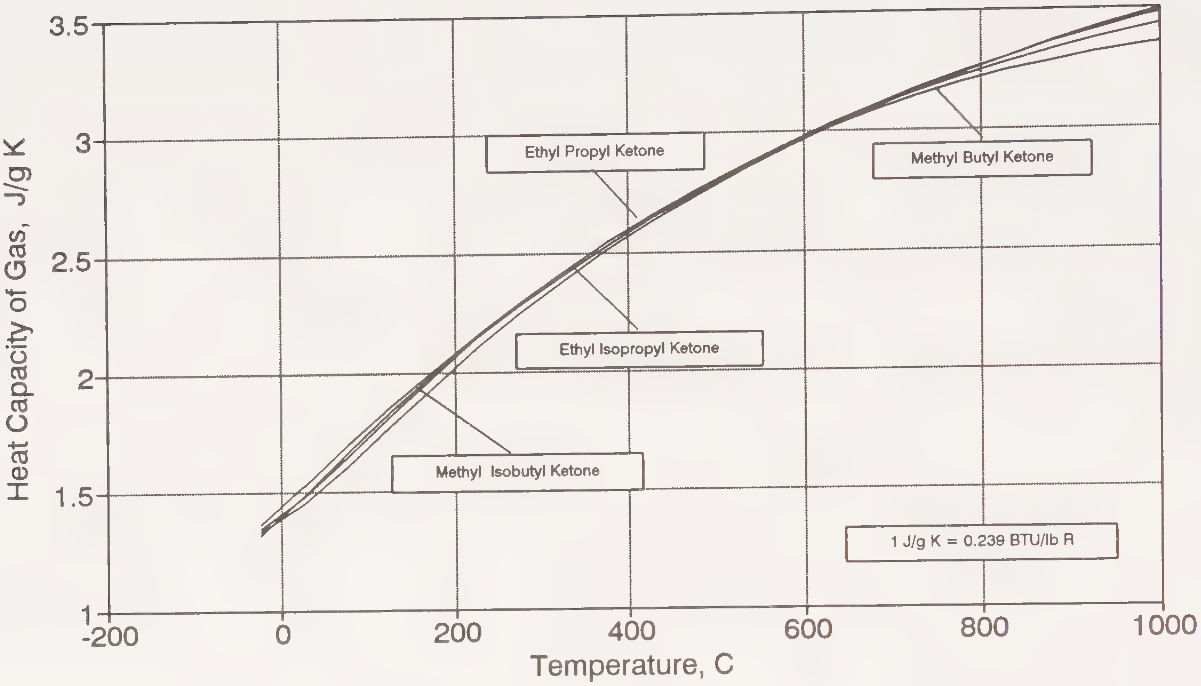

Figure 10-5 Heat Capacity of Gas

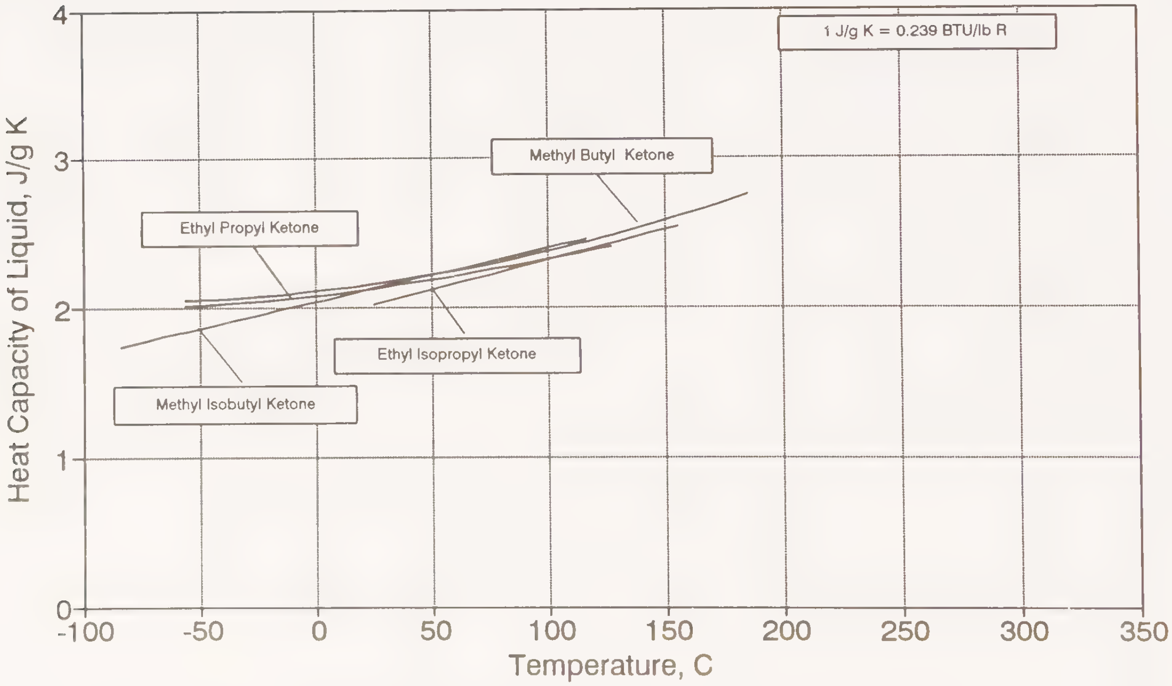

Figure 10-6 Heat Capacity of Liquid

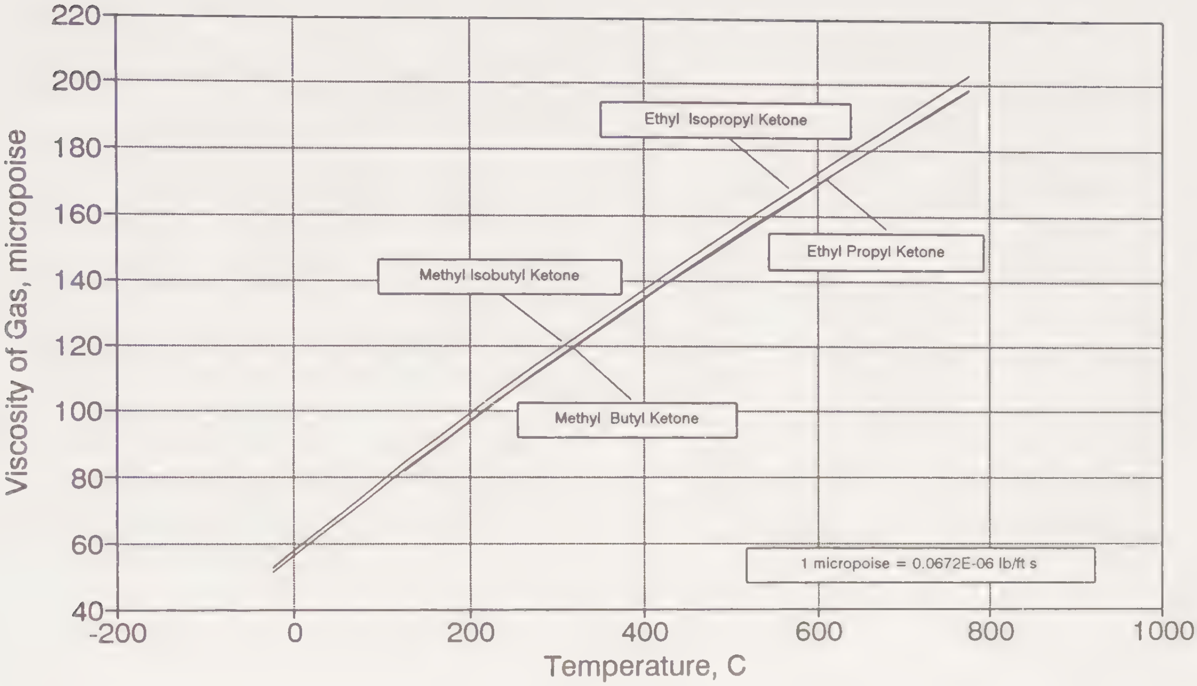

Figure 10-7 Viscosity of Gas

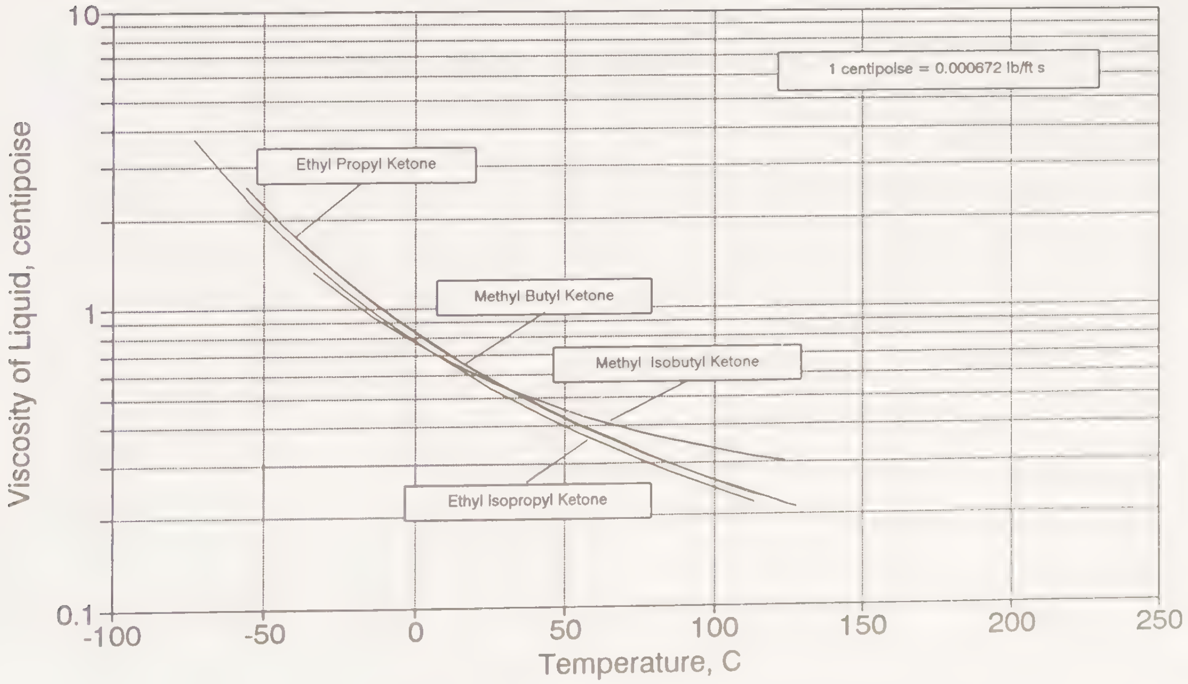

Figure 10-8 Viscosity of Liquid

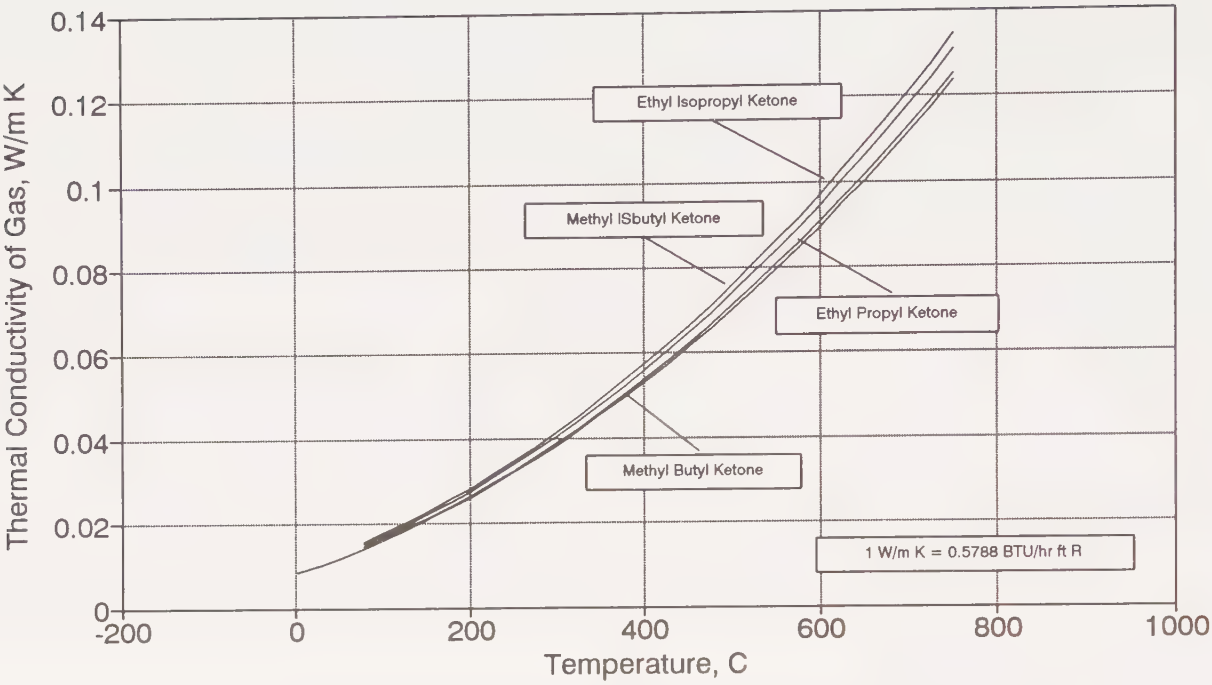

Figure 10-9 Thermal Conductivity of Gas

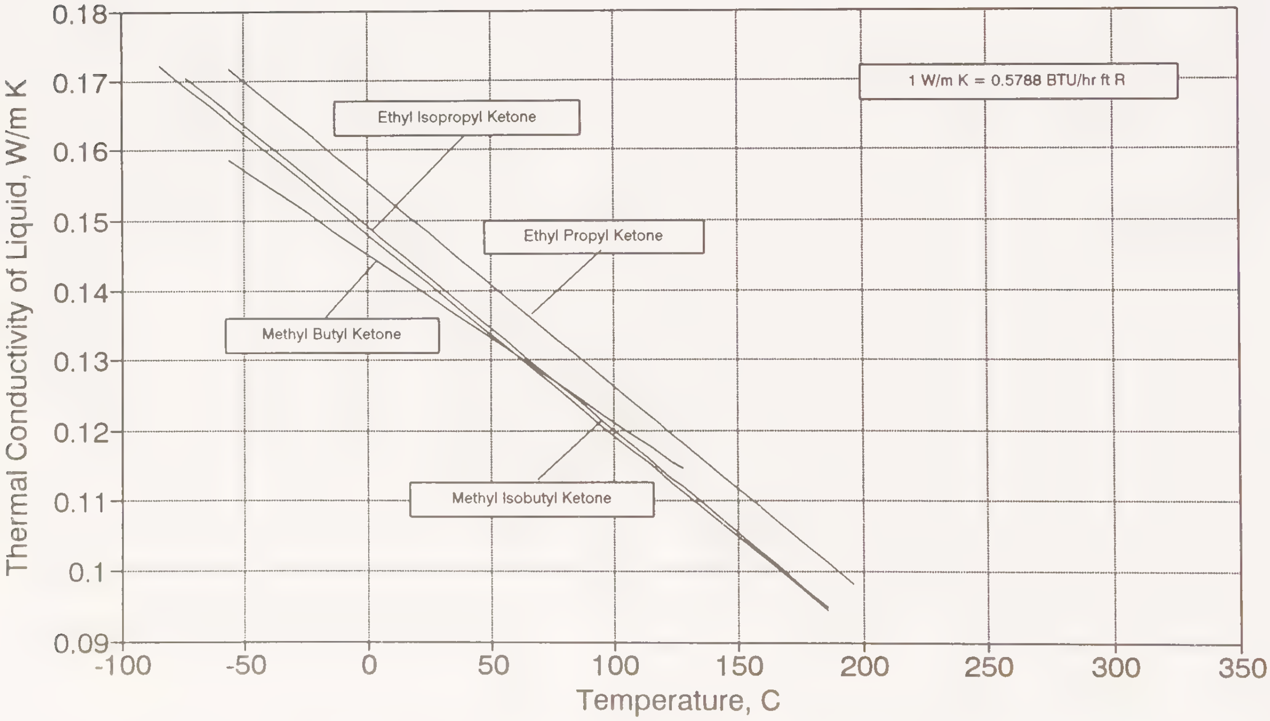

Figure 10-10 Thermal Conductivity of Liquid

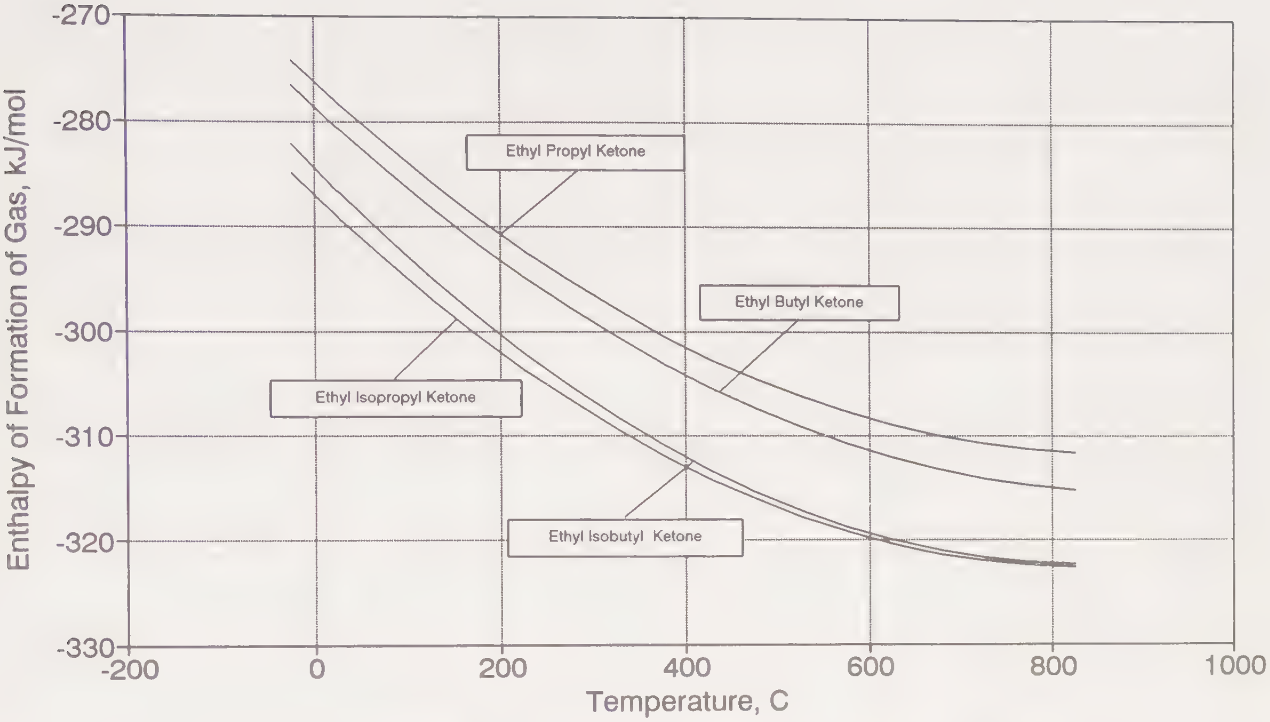

Figure 10-11 Enthalpy of Formation of Gas

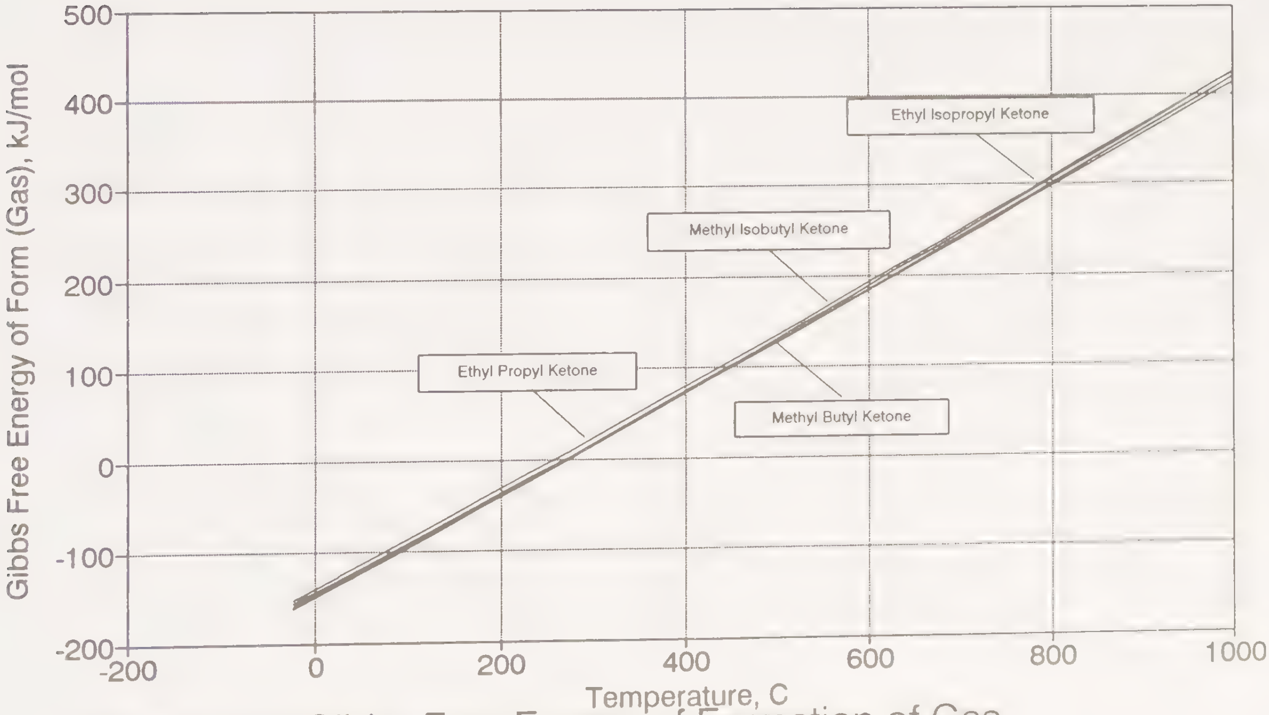

Figure 10-12 Gibbs Free Energy of Formation of Gas

Chapter 11

C_5 ETHERS

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 11-1

Property data from the literature (2,3,8,33-36,63-68,75,82-90,155-161) are given in Table 11-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 11-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 11-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 5%.

LIQUID DENSITY - Figure 11-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 5% in most cases.

SURFACE TENSION - Figure 11-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 11-5 and 11-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 5% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 3% or less in most cases except for methyl sec-butyl ether (possible 25% error).

VISCOSITY - Figures 11-7 and 11-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 5% or less in most cases except for methyl sec-butyl ether (possible 25% error).

THERMAL CONDUCTIVITY - Figures 11-9 and 11-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 10% in most cases except for methyl sec-butyl ether (possible 25% error).

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 11-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 11-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 11-1 Physical Properties

1. Name	Methyl tert-Butyl Ether	Methyl sec-Butyl Ether	Ethyl Propyl Ether
2. Formula	C5H12O	C5H12O	C5H12O
3. Molecular Weight, g/mol	88.150	88.150	88.150
4. Critical Temperature, K	497.10	498.00	500.23
5. Critical Pressure, bar	34.300	34.100	33.700
6. Critical Volume, ml/mol	329.00	329.00	339.00
7. Critical Compressibility Factor	0.273	0.271	0.275
8. Acentric Factor	0.2674	0.3062	0.3462
9. Melting Point, K	164.55	------	145.65
10. Boiling Point @ 1 atm, K	328.35	332.15	337.01
11. Heat of Vaporization @ BP, kJ/kg	319.61	327.68	312.86
12. Density of Liquid @ 25 C, g/ml	0.735	0.737	0.724
13. Surface Tension @ 25 C, dynes/cm	19.094	18.237	19.280
14. Heat Capacity of Gas @ 25 C, J/g K	1.450	1.551	1.536
15. Heat Capacity of Liquid @ 25 C, J/g K	2.127	2.168	2.238
16. Viscosity of Gas @ 25 C, micropoise	73.90	71.40	68.37
17. Viscosity of Liquid @ 25 C, centipoise	0.336	0.261	0.301
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.011	0.014	0.014
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.117	0.126	0.129
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-293.54	-275.63	-272.77
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-126.98	-118.22	-116.66
22. Flash Point, K	245.37	244.00	248.00
23. Autoignition Temperture, K	------	------	------
24. Lower Explosion Limit in Air, vol %	2.0	1.4	1.7
25. Upper Explosion Limit in Air, vol %	15.1	11.5	9.0
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

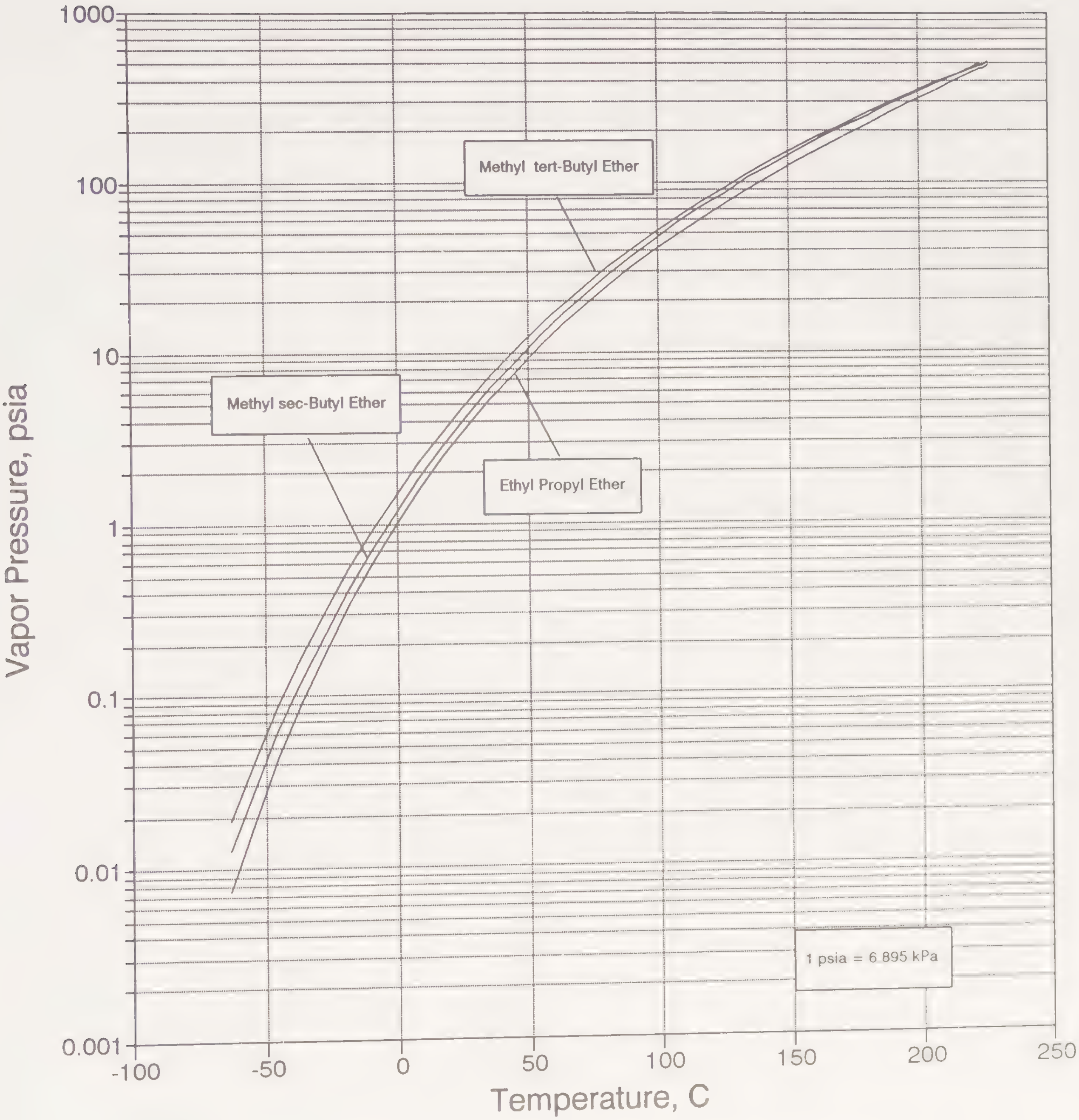

Figure 11-1 Vapor Pressure

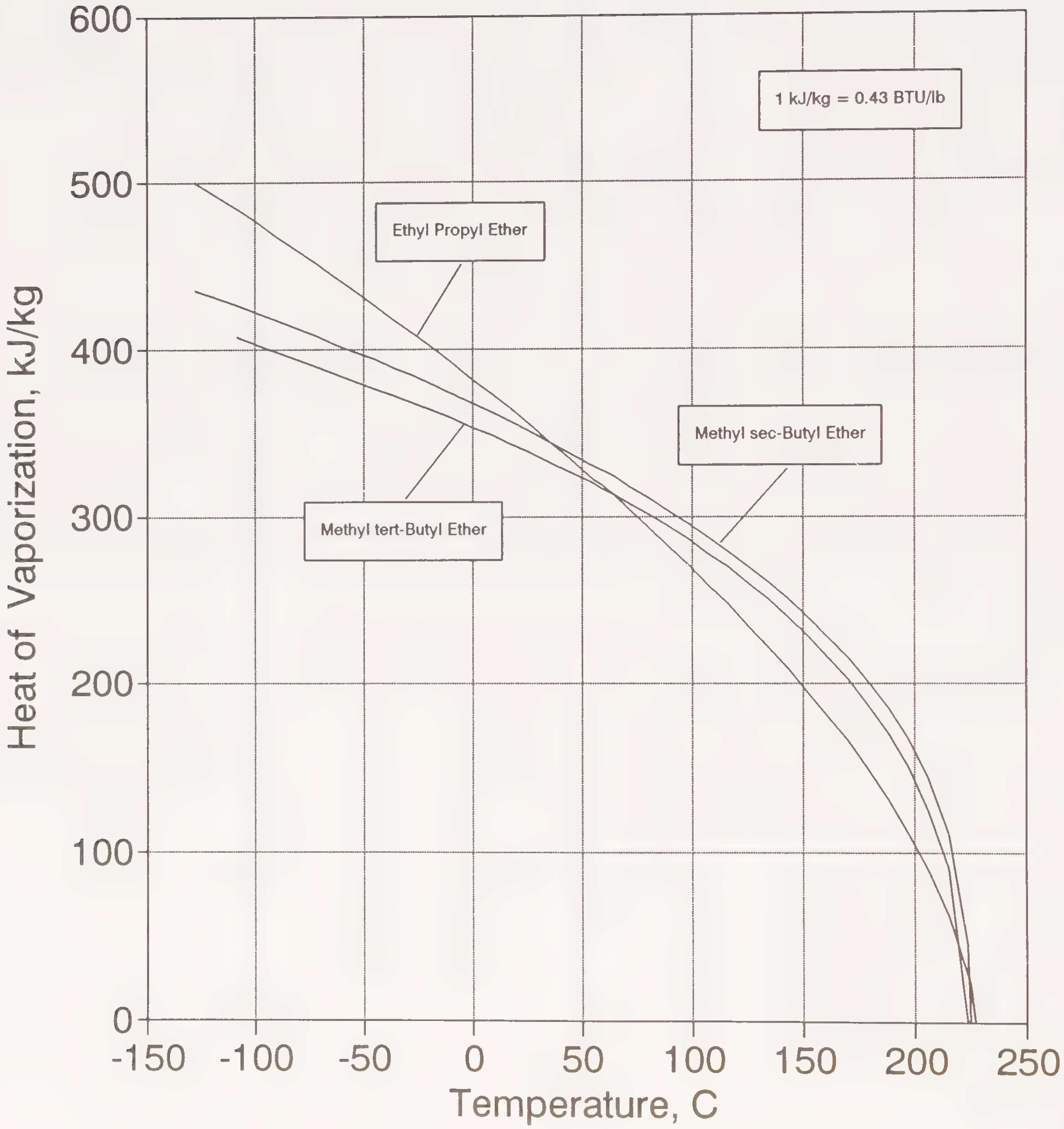

Figure 11-2 Heat of Vaporization

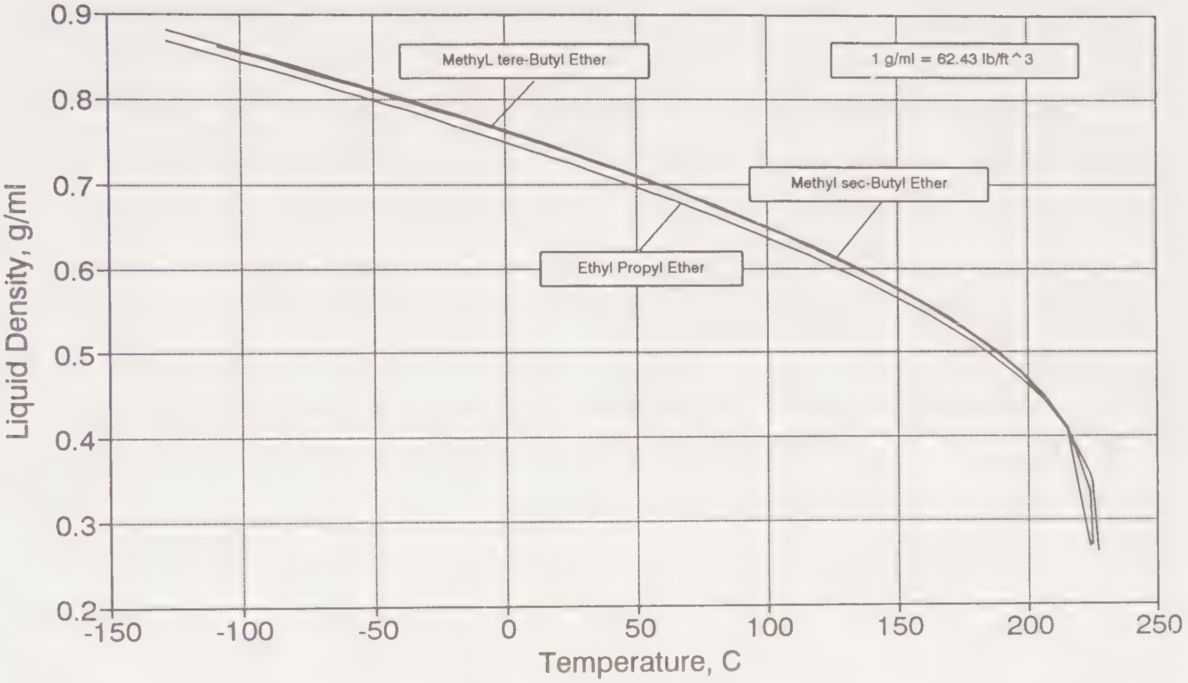

Figure 11-3 Liquid Density

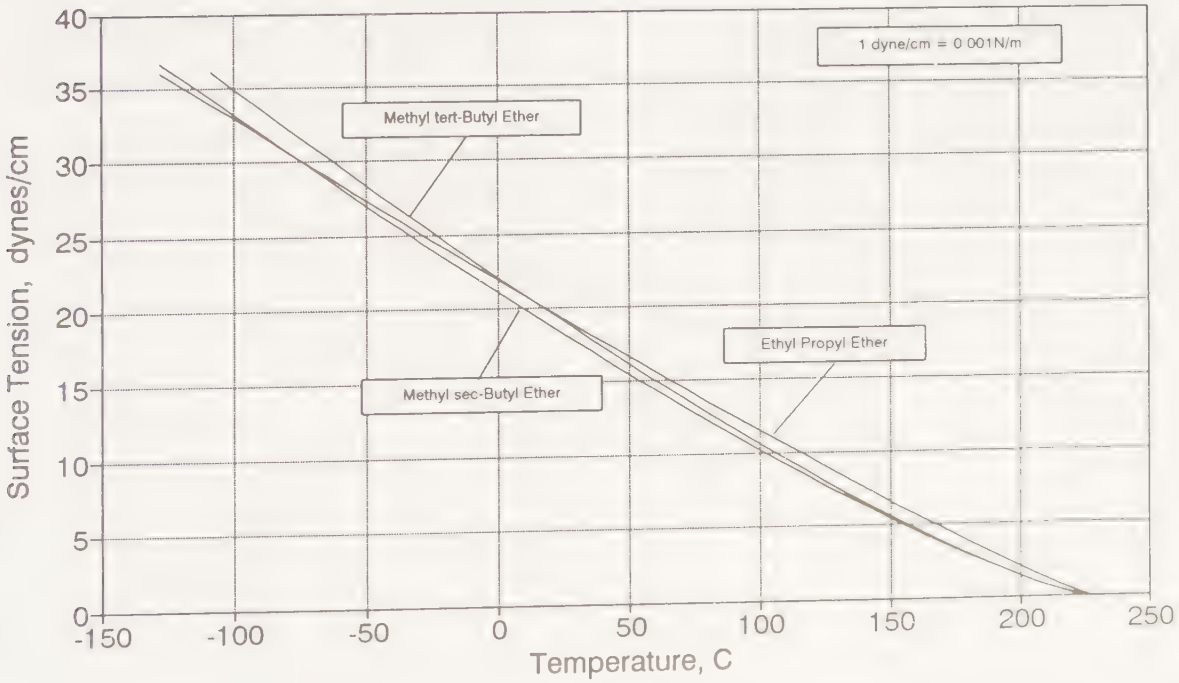

Figure 11-4 Surface Tension

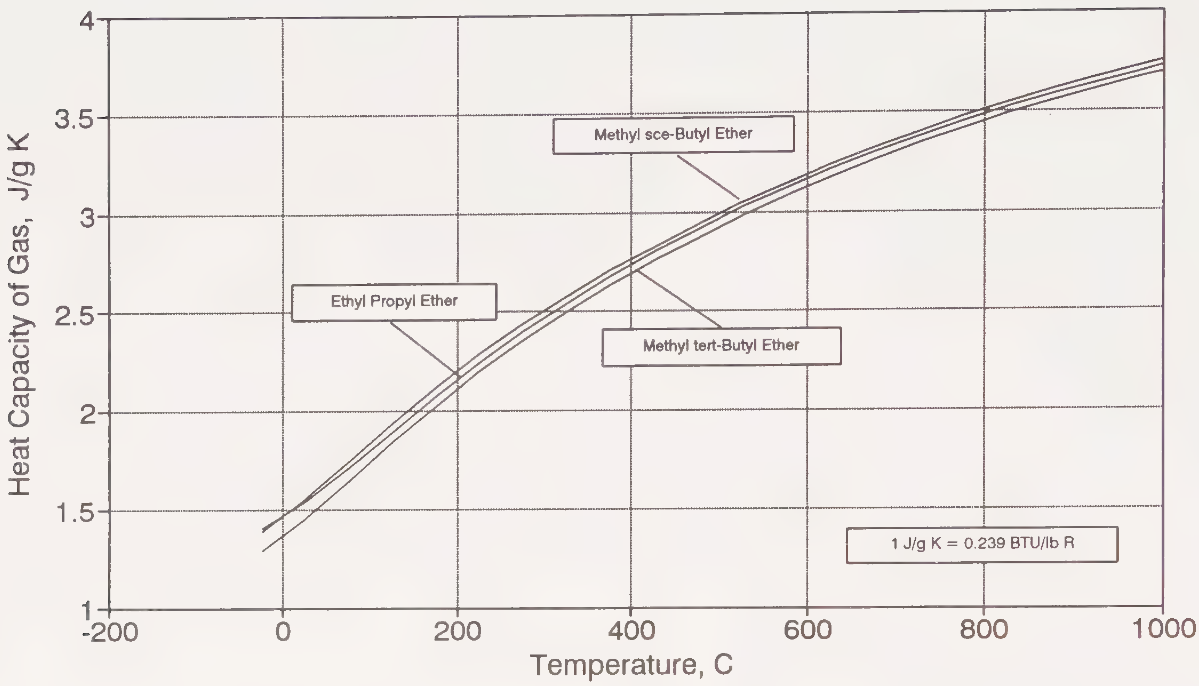

Figure 11-5 Heat Capacity of Gas

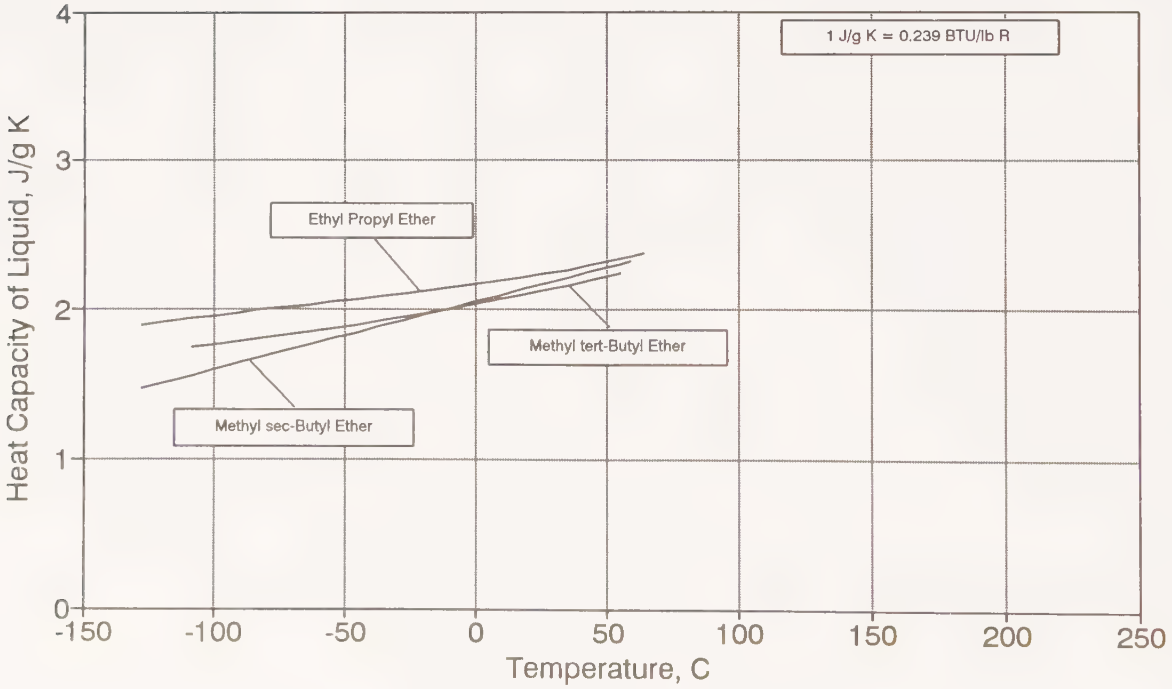

Figure 11-6 Heat Capacity of Liquid

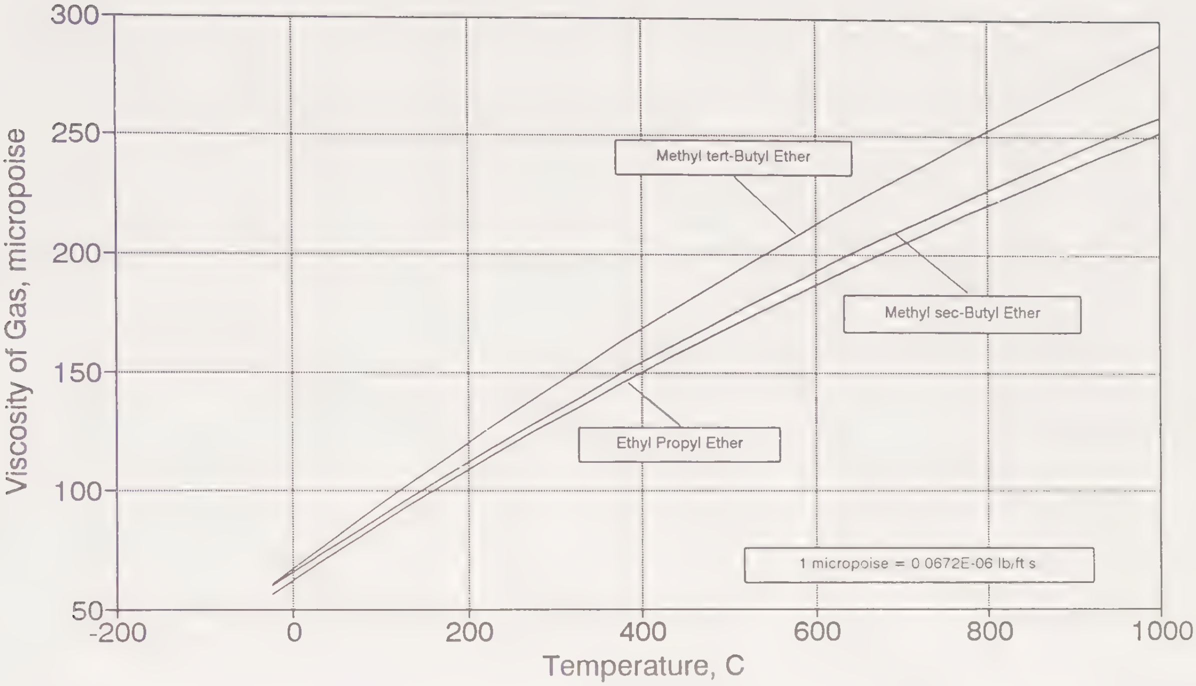

Figure 11-7 Viscosity of Gas

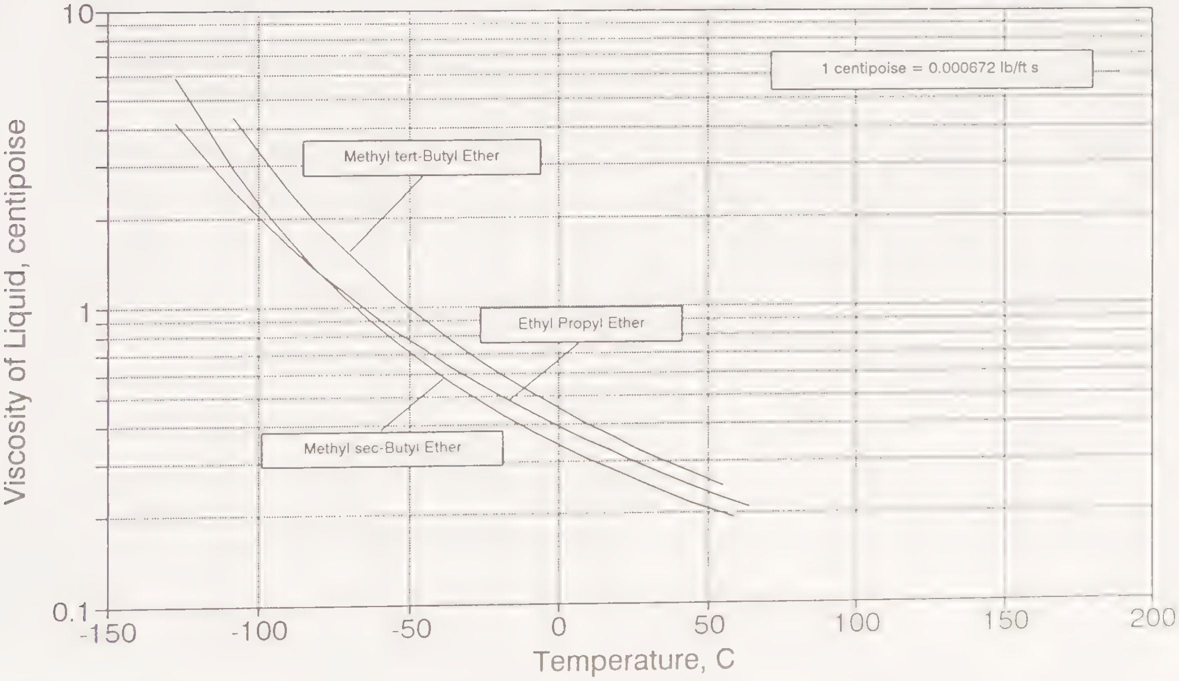

Figure 11-8 Viscosity of Liquid

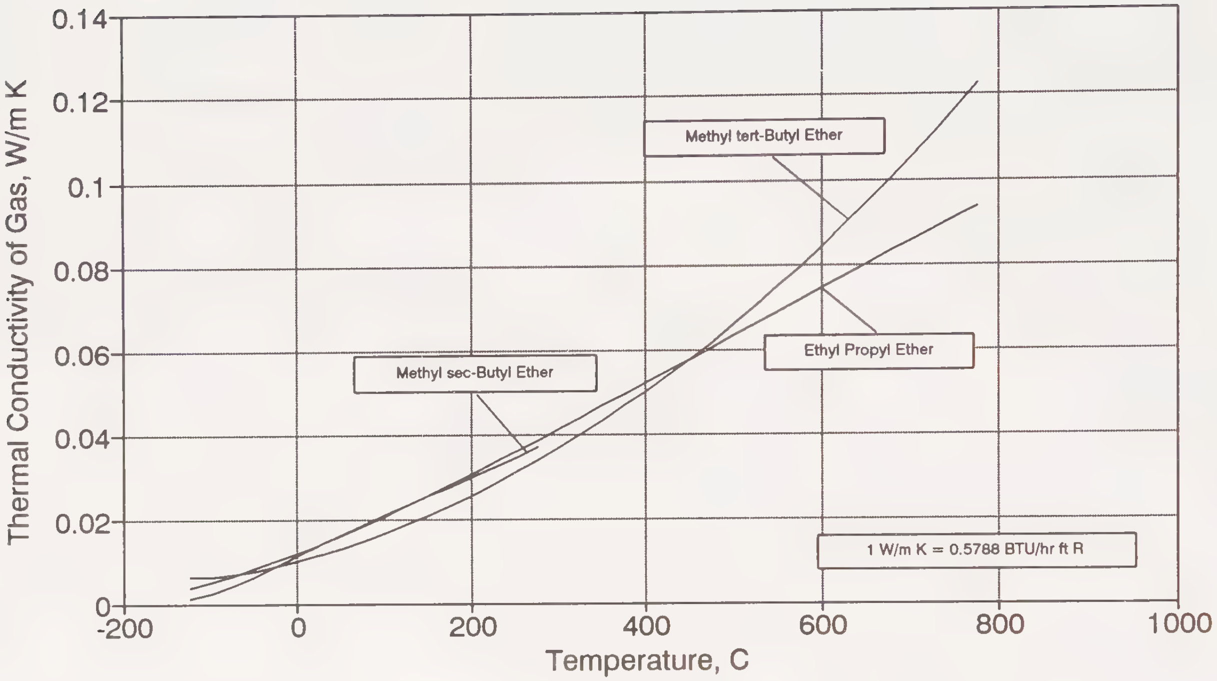

Figure 11-9 Thermal Conductivity of Gas

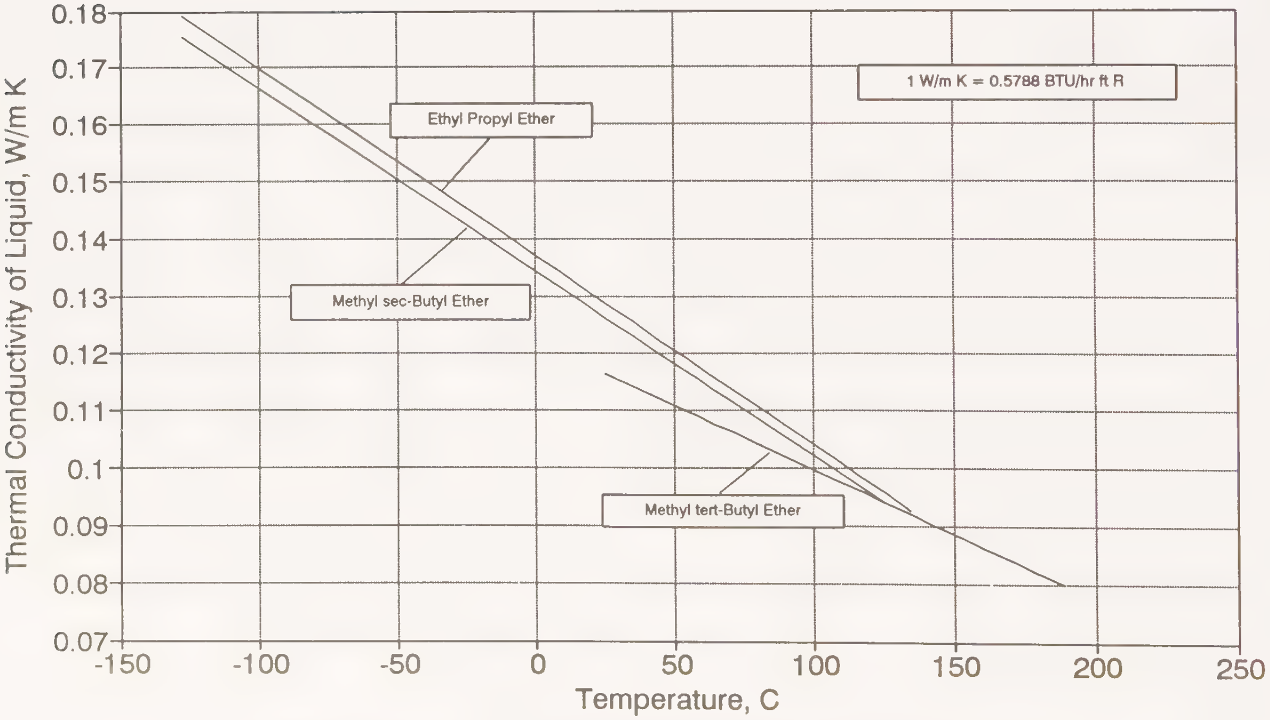

Figure 11-10 Thermal Conductivity of Liquid

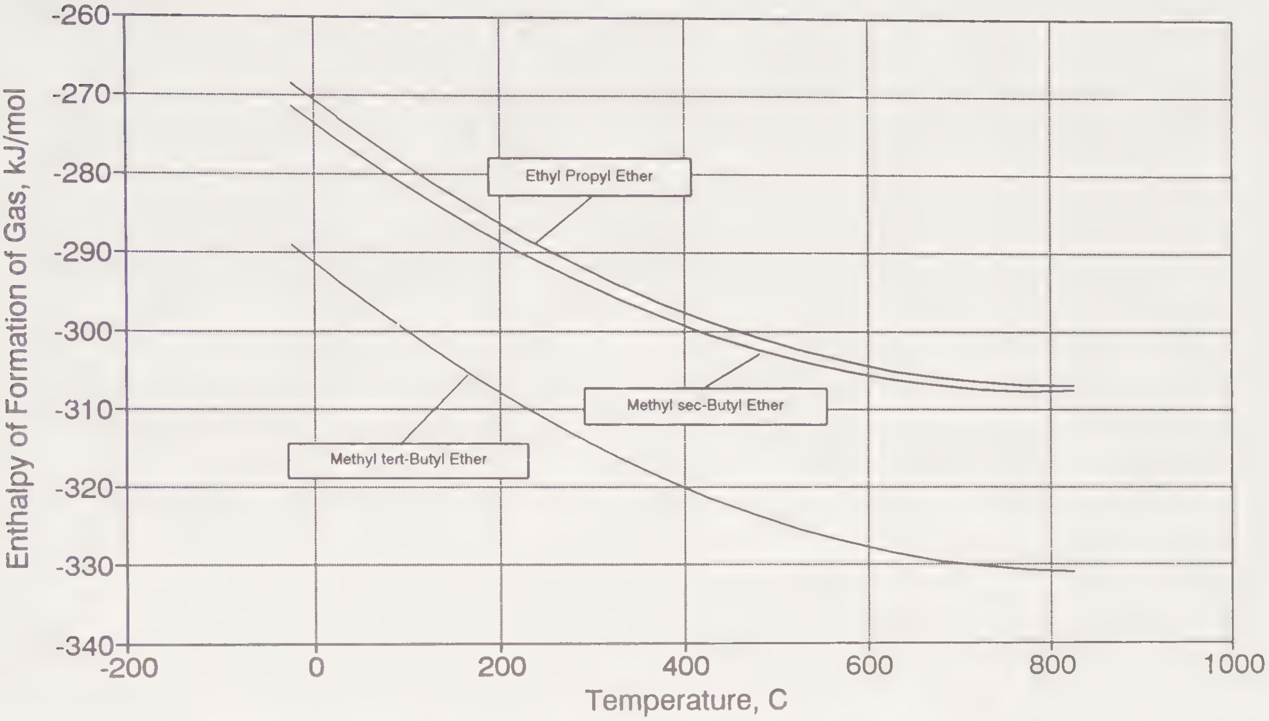

Figure 11-11 Enthalpy of Formation of Gas

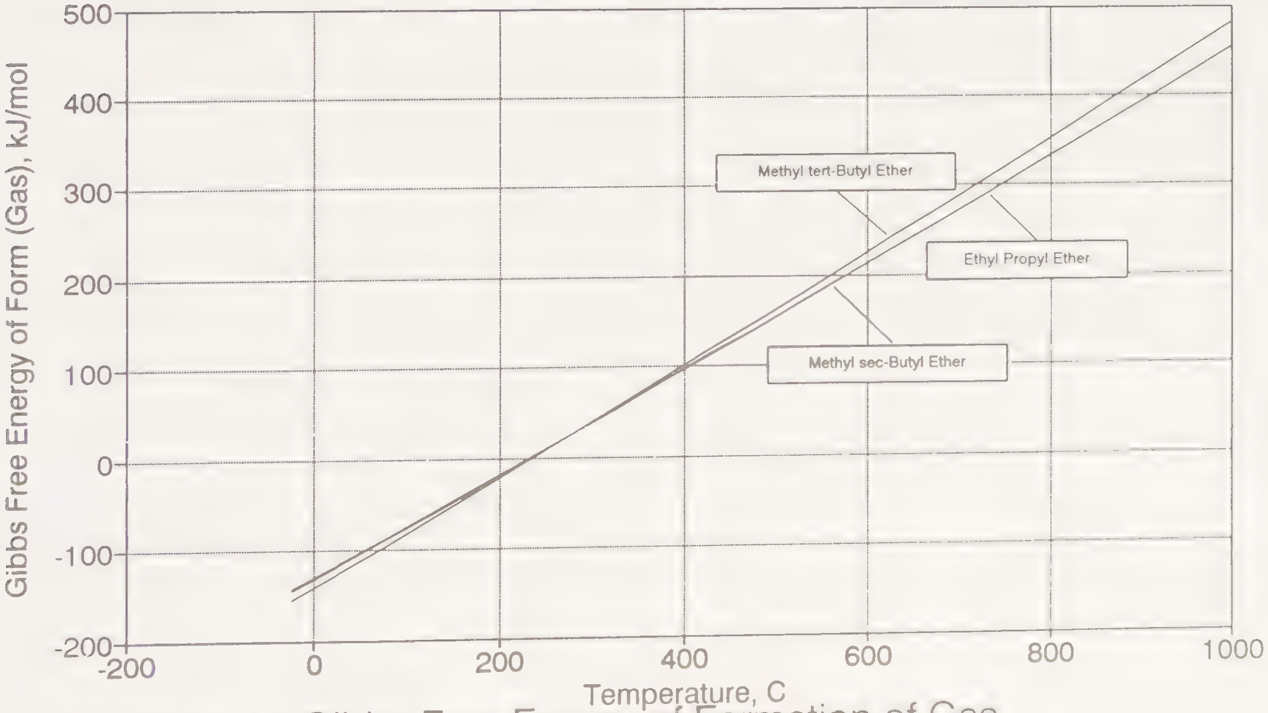

Figure 11-12 Gibbs Free Energy of Formation of Gas

Chapter 12

C_1 TO C_3 FORMATES

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 12-1

Property data from the literature (2,3,8,21-23,36-38,66,73-79,90,121,157, 179-182) are given in Table 12-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 12-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 3% or less in most cases.

HEAT OF VAPORIZATION - Figure 12-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 3%.

LIQUID DENSITY - Figure 12-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 1% in most cases.

SURFACE TENSION - Figure 12-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 3% or less in most cases.

HEAT CAPACITY - Figures 12-5 and 12-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 3% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in favorable agreement with data. Errors are about 5% or less in most cases. Heat capacity of liquid for ethyl formate was estimated using values for methyl formate and propyl formate.

VISCOSITY - Figures 12-7 and 12-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in favorable agreement with data. Errors are about 5% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 5% or less in most cases.

THERMAL CONDUCTIVITY - Figures 12-9 and 12-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is favorable with errors less then 5% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is favorable with possible errors of 5% in most cases.

ENTHALPY OF FORMATION - Figure 12-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 12-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 12-1 Physical Properties

1. Name	Methyl Formate	Ethyl Formate	Propyl Formate
2. Formula	C2H4O2	C3H6O2	C4H8O2
3. Molecular Weight, g/mol	60.053	74.079	88.106
4. Critical Temperature, K	487.20	508.40	538.00
5. Critical Pressure, bar	59.984	47.420	40.631
6. Critical Volume, ml/mol	172.00	229.00	285.00
7. Critical Compressibility Factor	0.255	0.257	0.259
8. Acentric Factor	0.2537	0.2849	0.3180
9. Melting Point, K	174.15	193.55	180.25
10. Boiling Point @ 1 atm, K	304.90	327.46	353.97
11. Heat of Vaporization @ BP, kJ/kg	496.35	402.08	363.27
12. Density of Liquid @ 25 C g/ml	0.967	0.917	0.900
13. Surface Tension @ 25 C, dynes/cm	24.244	23.084	23.945
14. Heat Capacity of Gas @ 25 C, J/g K	1.096	1.208	1.251
15. Heat Capacity of Liquid @ 25 C, J/g K	1.983	1.958	1.933
16. Viscosity of Gas @ 25 C, micropoise	94.13	84.27	76.84
17. Viscosity of Liquid @ 25 C, centipoise	0.330	0.380	0.486
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.014	0.011	0.010
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.184	0.160	0.147
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-352.75	-388.58	-404.98
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-295.54	-303.94	-292.87
22. Flash Point, K	254.26	269.15	270.37
23. Autoignition Temperture, K	729.26	728.15	728.15
24. Lower Explosion Limit in Air, vol %	5.9	2.7	2.1
25. Upper Explosion Limit in Air, vol %	20.0	13.5	11.3
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

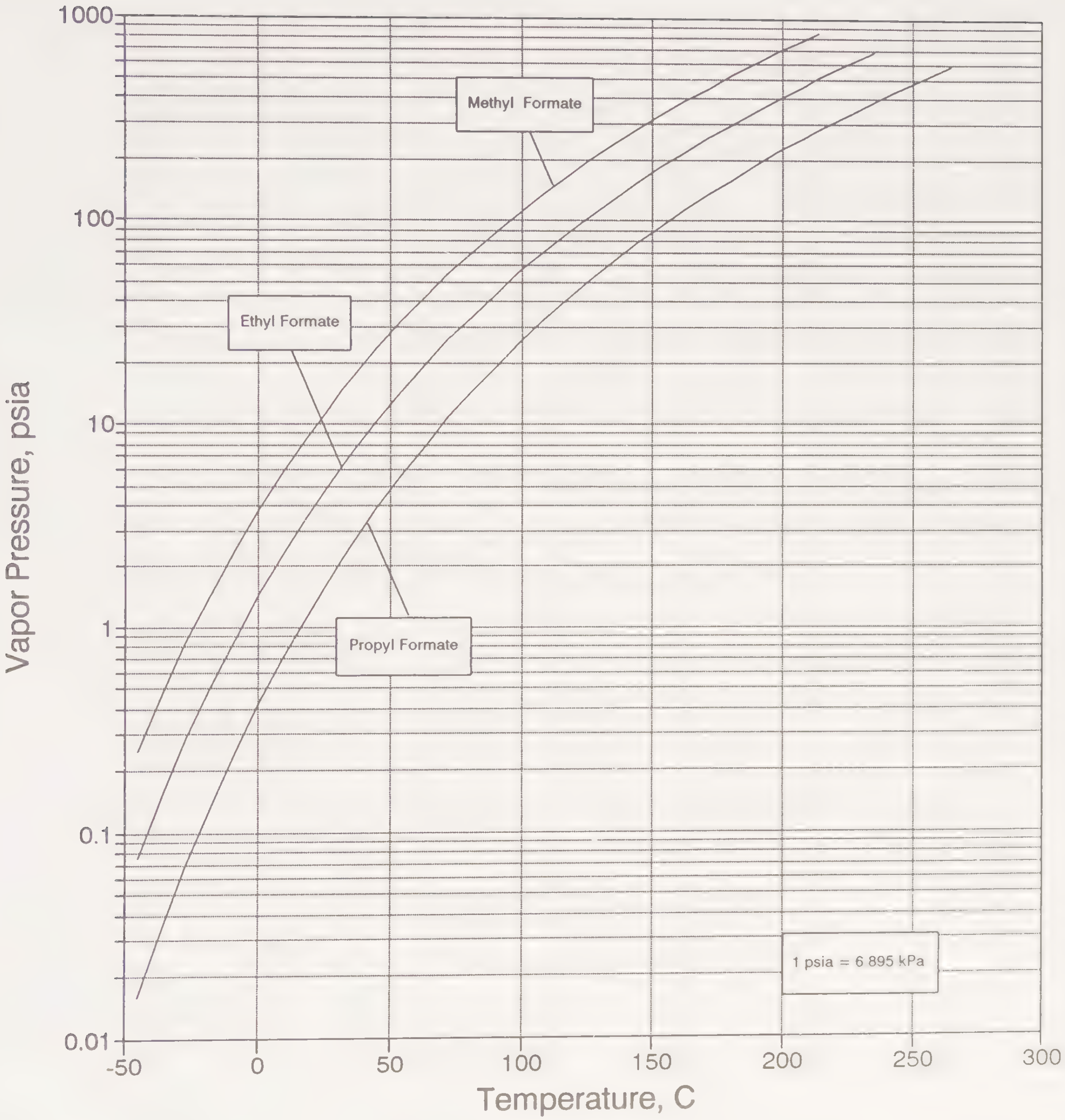

Figure 12-1 Vapor Pressure

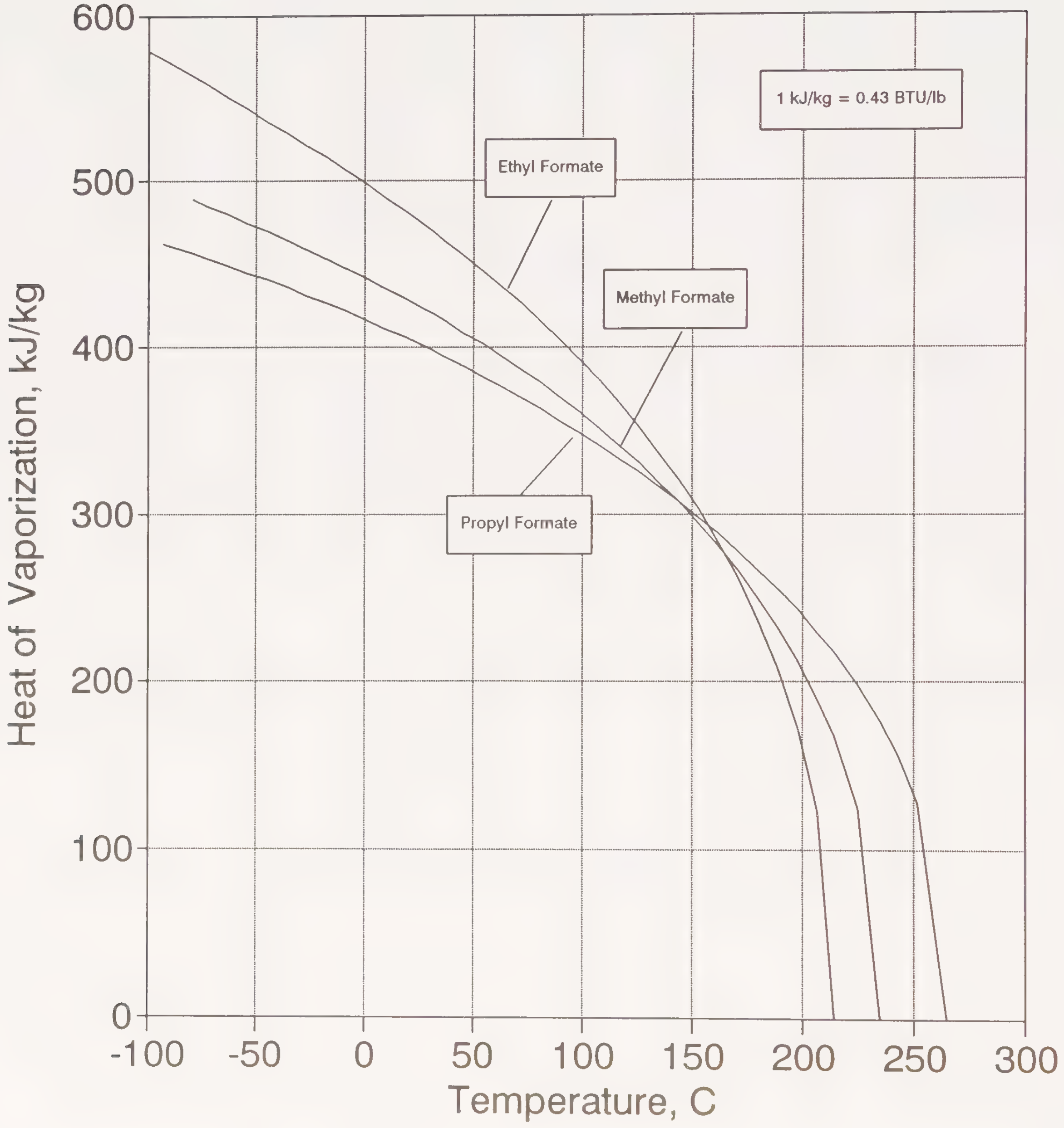

Figure 12-2 Heat of Vaporization

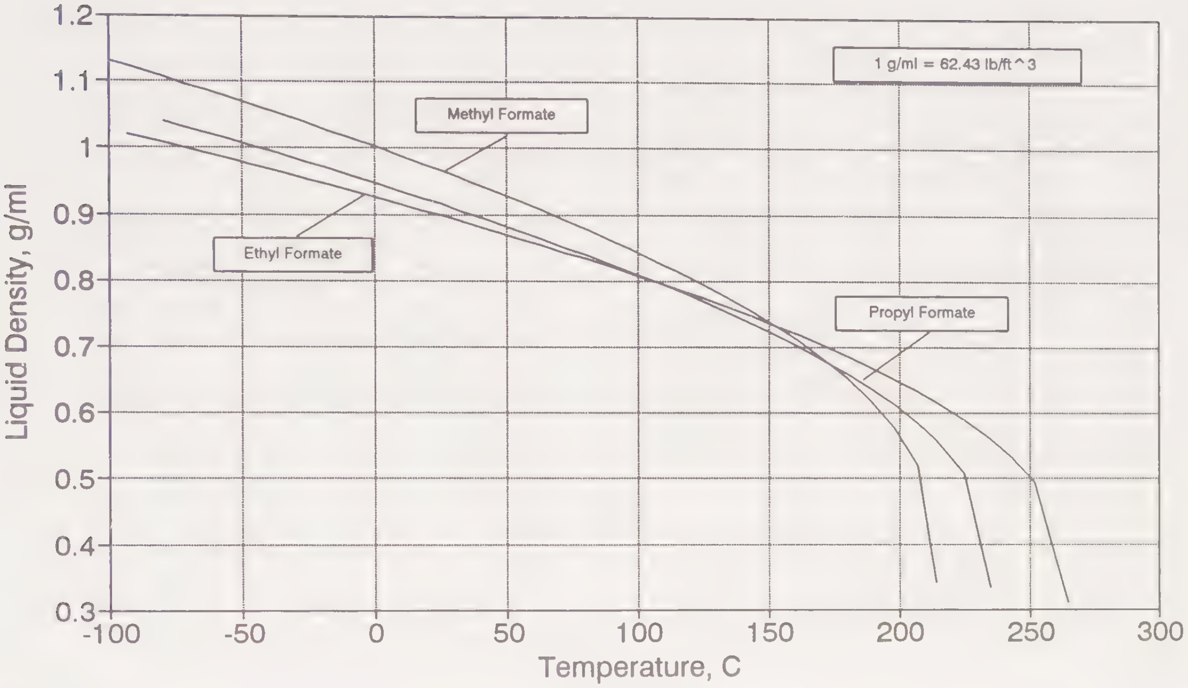

Figure 12-3 Liquid Density

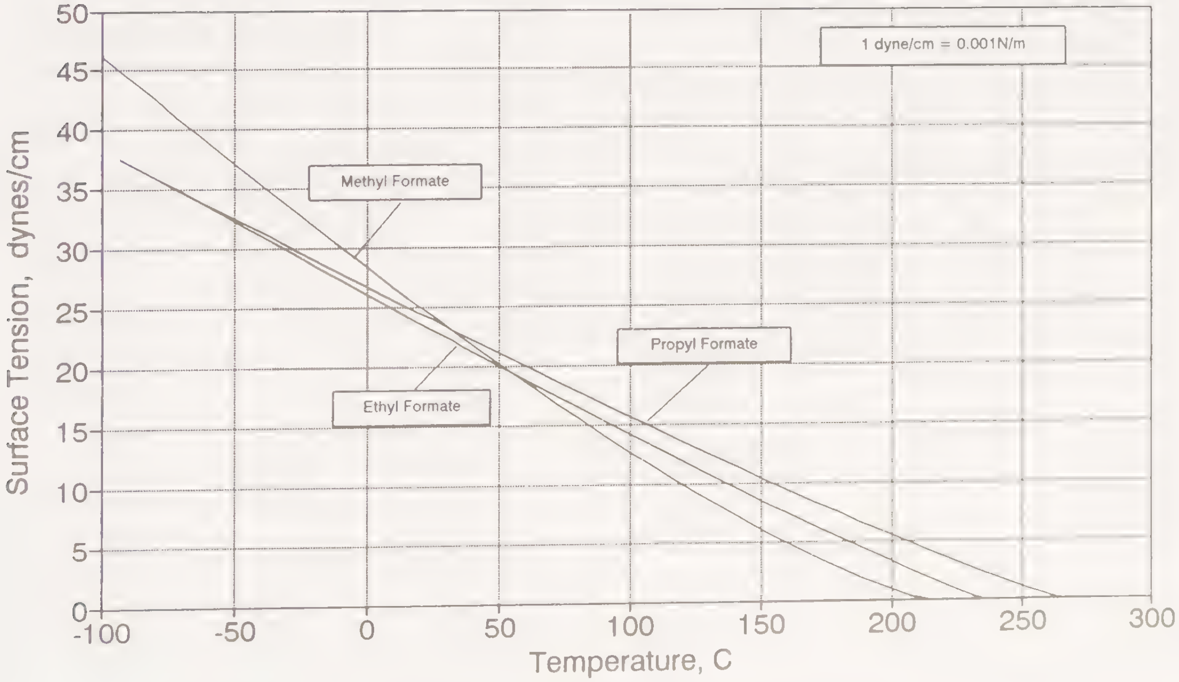

Figure 12-4 Surface Tension

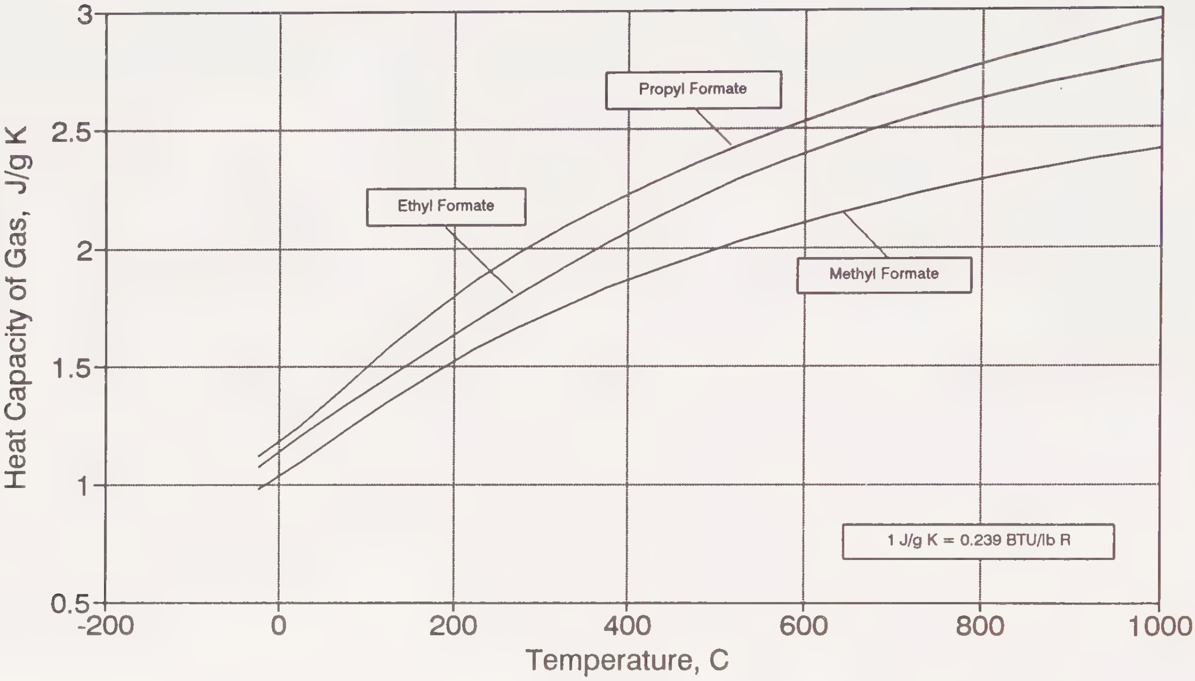

Figure 12-5 Heat Capacity of Gas

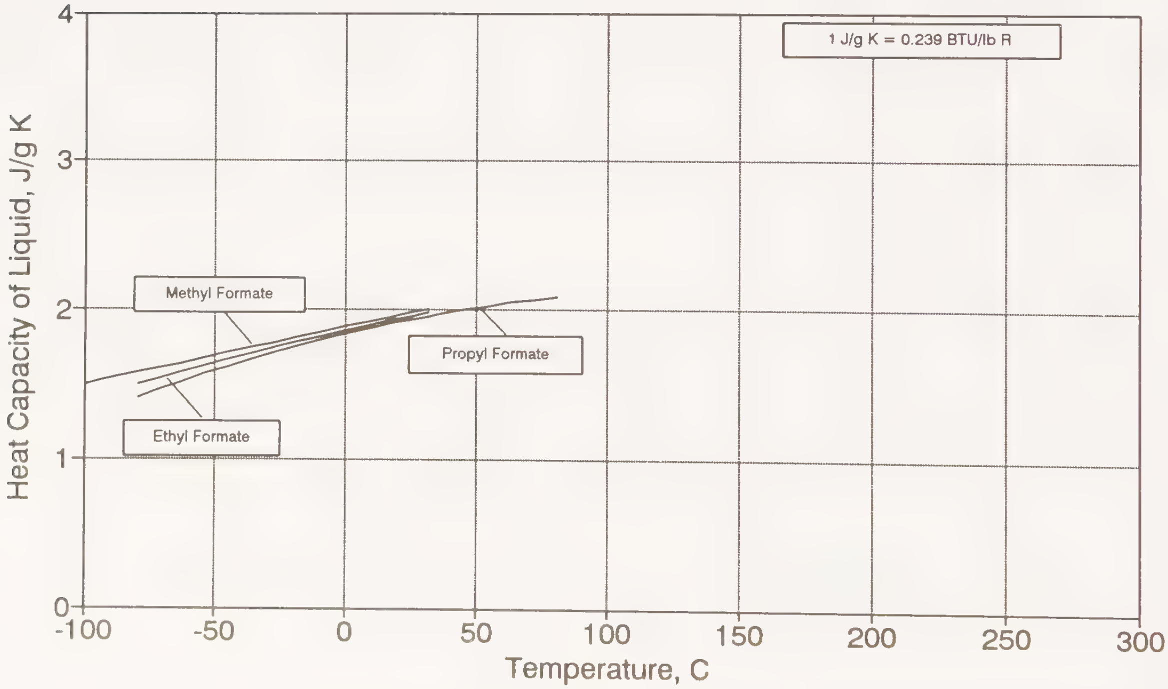

Figure 12-6 Heat Capacity of Liquid

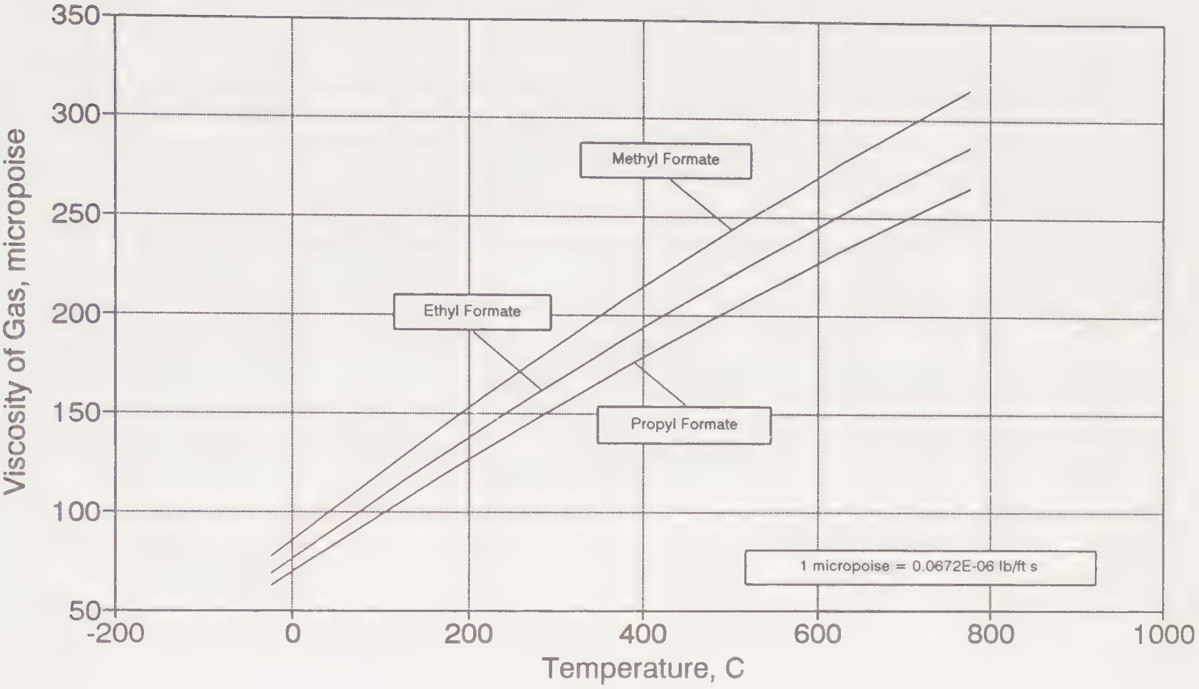

Figure 12-7 Viscosity of Gas

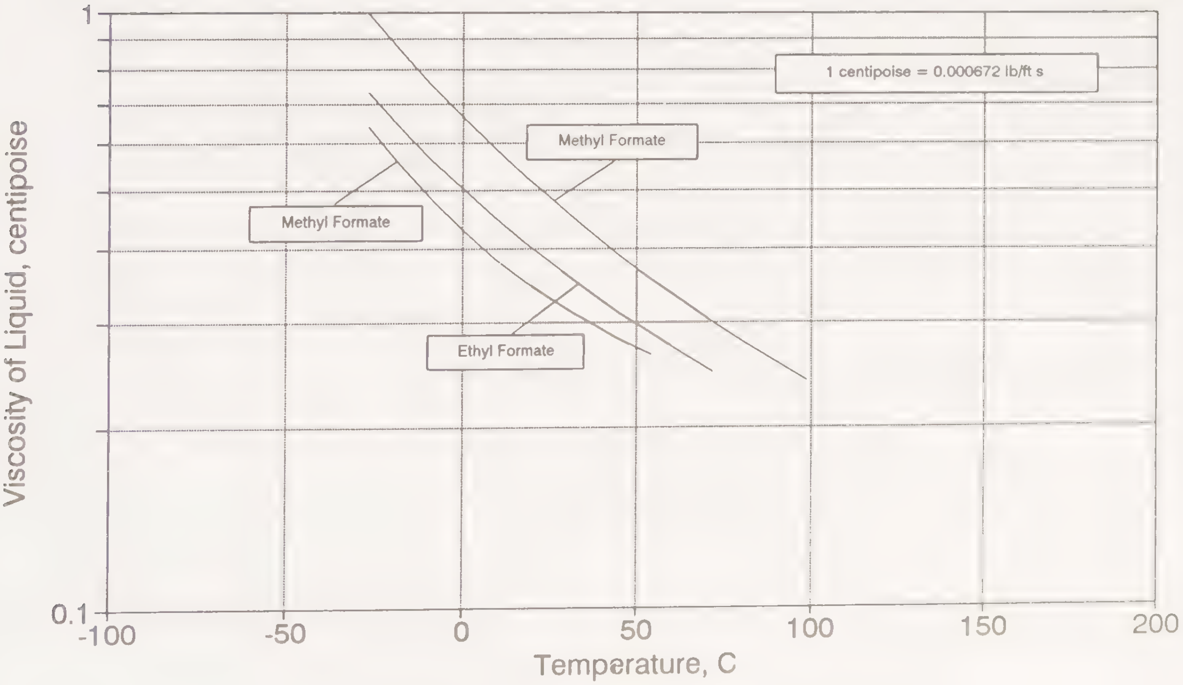

Figure 12-8 Viscosity of Liquid

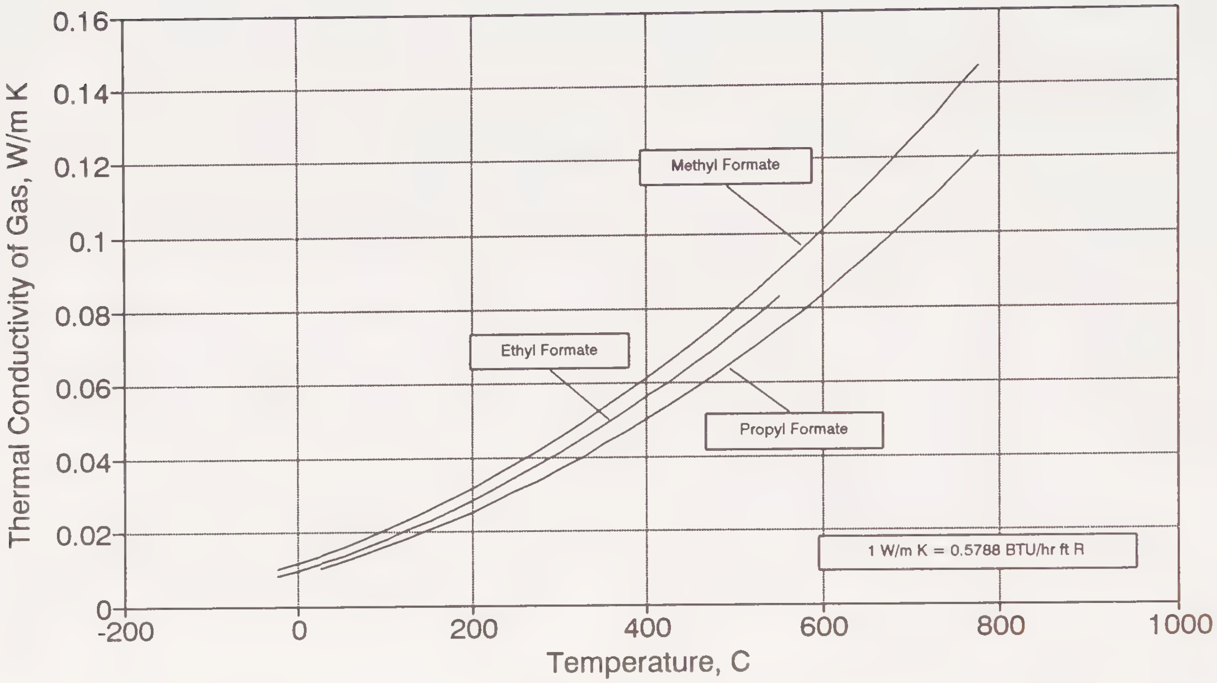

Figure 12-9 Thermal Conductivity of Gas

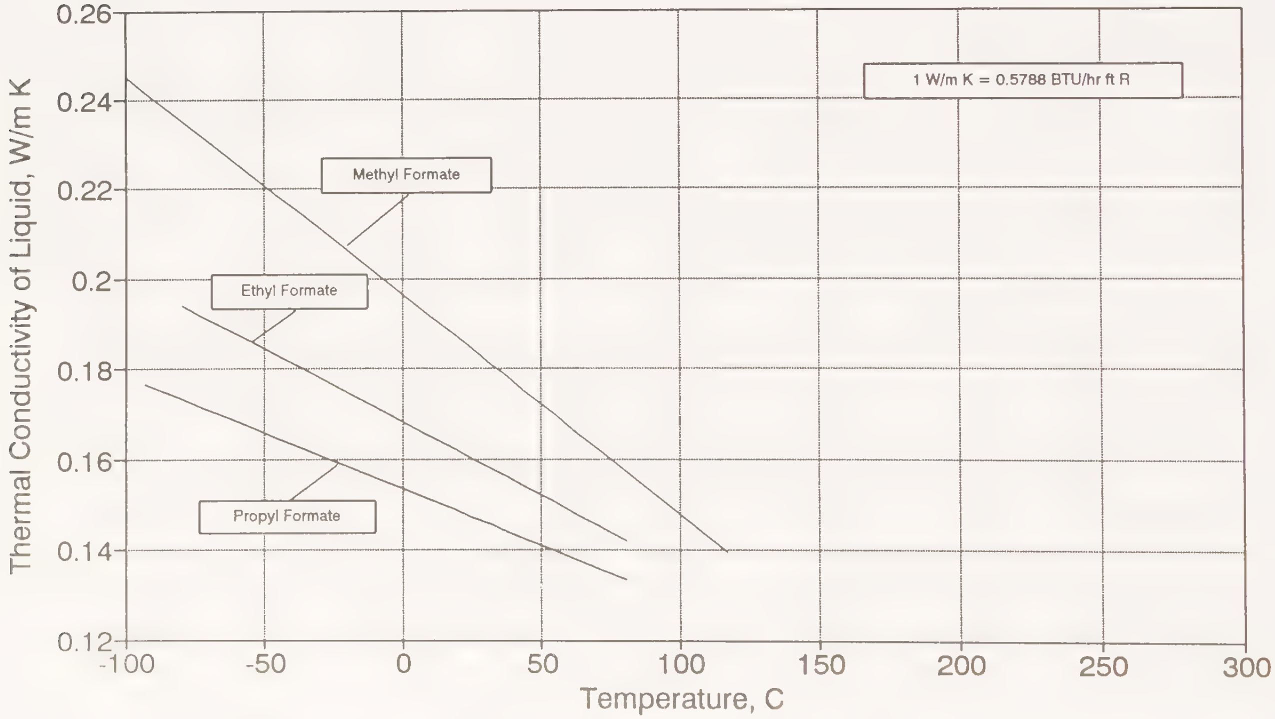

Figure 12-10 Thermal Conductivity of Liquid

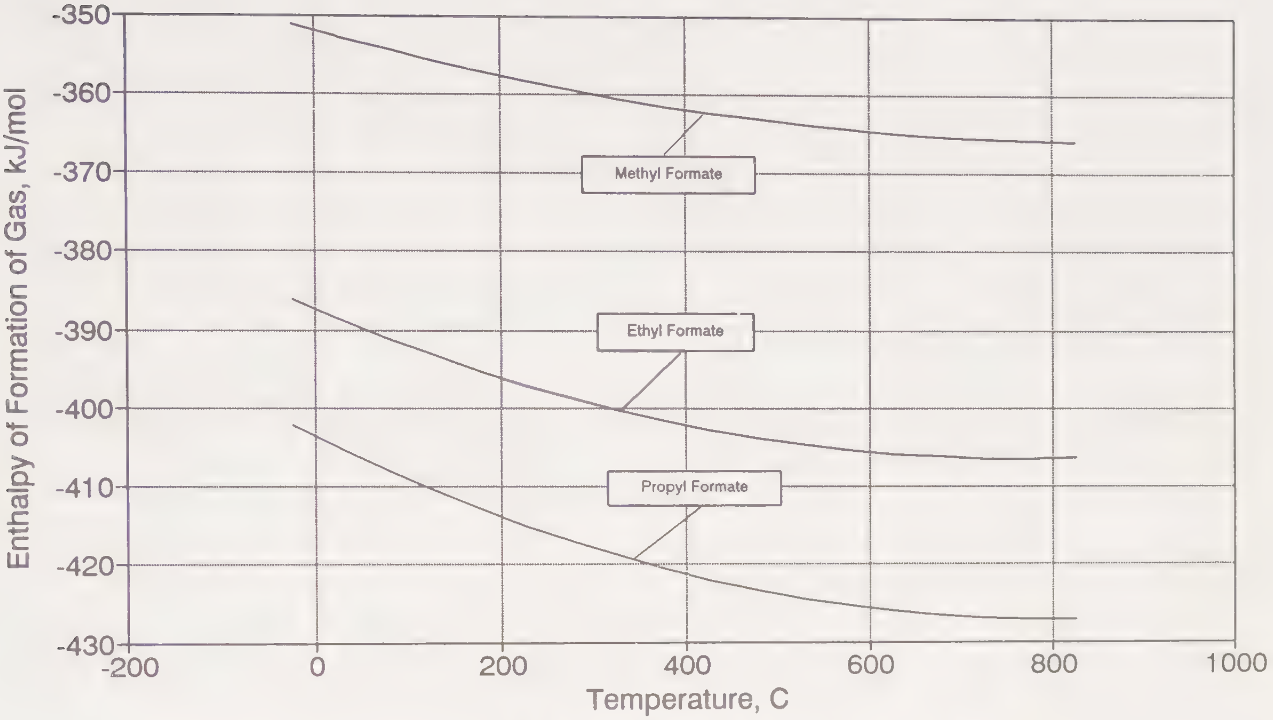

Figure 12-11 Enthalpy of Formation of Gas

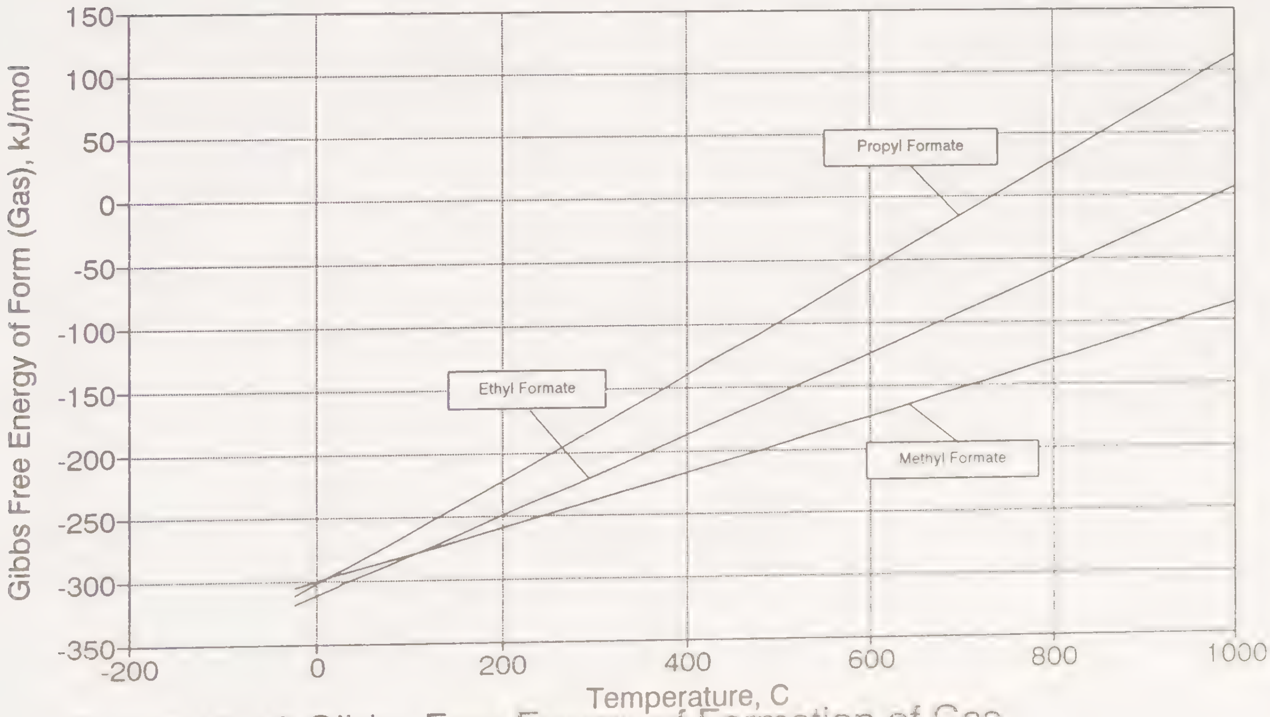

Figure 12-12 Gibbs Free Energy of Formation of Gas

Chapter 13

C_4 FORMATES

Robert W. Gallant, Carl L. Yaws and Xiaoyan Lin

PHYSICAL PROPERTIES - Table 13-1

Property data from the literature (2,3,8,33-36,62-66,70-73,79,90,103,109,155,157) are given in Table 13-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 13-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 3% or less in most cases.

HEAT OF VAPORIZATION - Figure 13-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with possible errors of 3%.

LIQUID DENSITY - Figure 13-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 1% in most cases.

SURFACE TENSION - Figure 13-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 3% or less in most cases.

HEAT CAPACITY - Figures 13-5 and 13-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are with errors of 3% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are favorable with errors of 5% or less in most cases.

VISCOSITY - Figures 13-7 and 13-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in favorable agreement with data. Errors are about 5% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 5% or less in most cases.

THERMAL CONDUCTIVITY - Figures 13-9 and 13-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is favorable with possible errors of 5% in most cases.

ENTHALPY OF FORMATION - Figure 13-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 13-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 13-1 Physical Properties

1. Name	Isobutyl Formate	Butyl Formate
2. Formula	C5H10O2	C5H10O2
3. Molecular Weight, g/mol	102.133	102.133
4. Critical Temperature, K	551.35	559.00
5. Critical Pressure, bar	38.808	35.100
6. Critical Volume, ml/mol	352.00	336.00
7. Critical Compressibility Factor	0.298	0.254
8. Acentric Factor	0.3896	0.3844
9. Melting Point, K	177.35	181.25
10. Boiling Point @ 1 atm, K	371.22	379.25
11. Heat of Vaporization @ BP, kJ/kg	332.69	352.21
12. Density of Liquid @ 25 C, g/ml	0.875	0.887
13. Surface Tension @ 25 C, dynes/cm	23.210	24.523
14. Heat Capacity of Gas @ 25 C, J/g K	1.309	1.307
15. Heat Capacity of Liquid @ 25 C, J/g K	2.116	1.934
16. Viscosity of Gas @ 25 C, micropoise	73.809	74.623
17. Viscosity of Liquid @ 25 C, centipoise	0.617	0.645
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.014	0.010
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.142	0.142
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-437.04	-425.79
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-294.40	-284.87
22. Flash Point, K	277.00	290.93
23. Autoignition Temperature, K	593.15	595.37
24. Lower Explosion Limit in Air, vol %	1.7	1.7
25. Upper Explosion Limit in Air, vol %	8.0	8.0
26. Solubility in Water @ 25 C, ppm(wt)	------	------

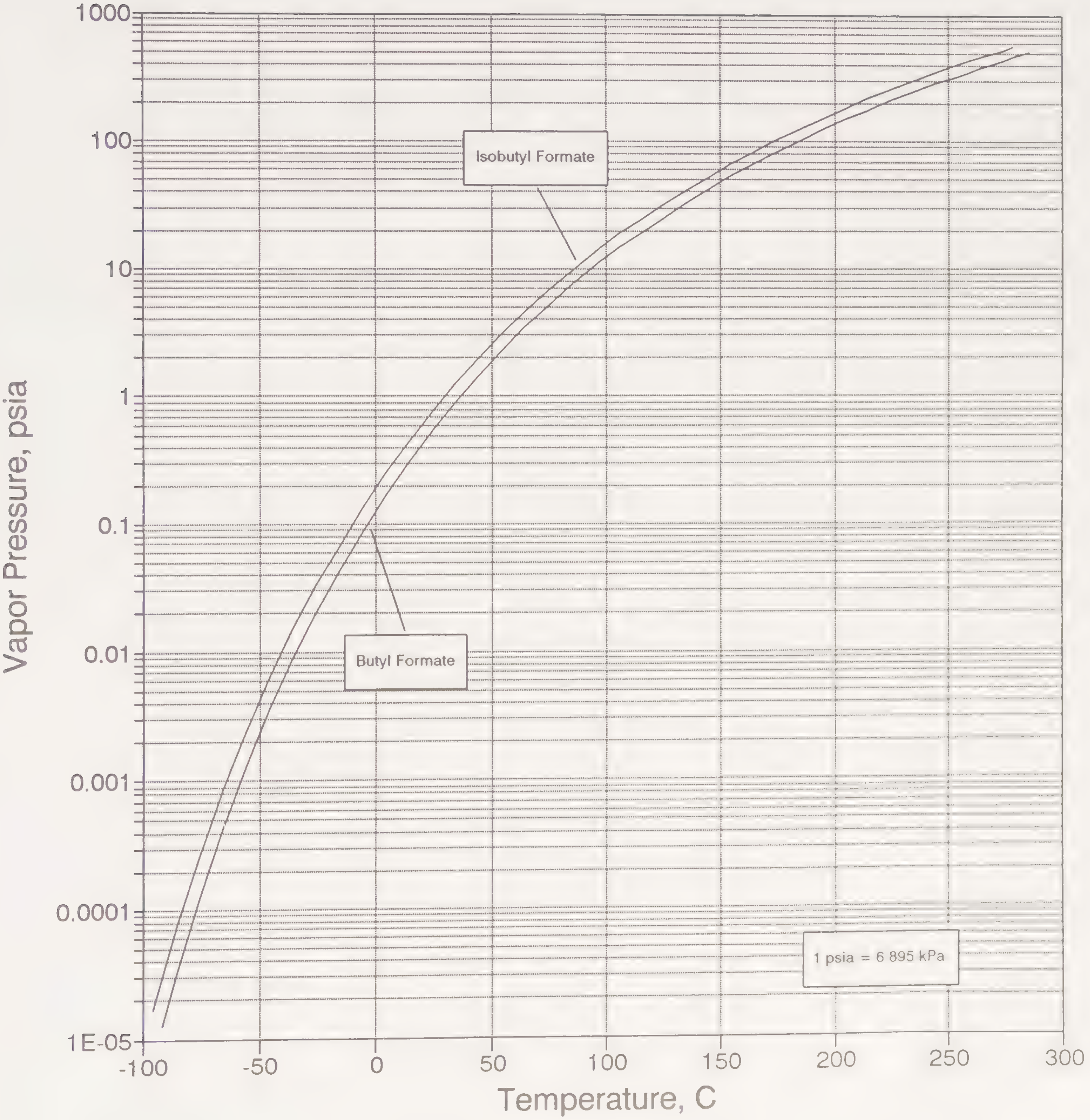

Figure 13-1 Vapor Pressure

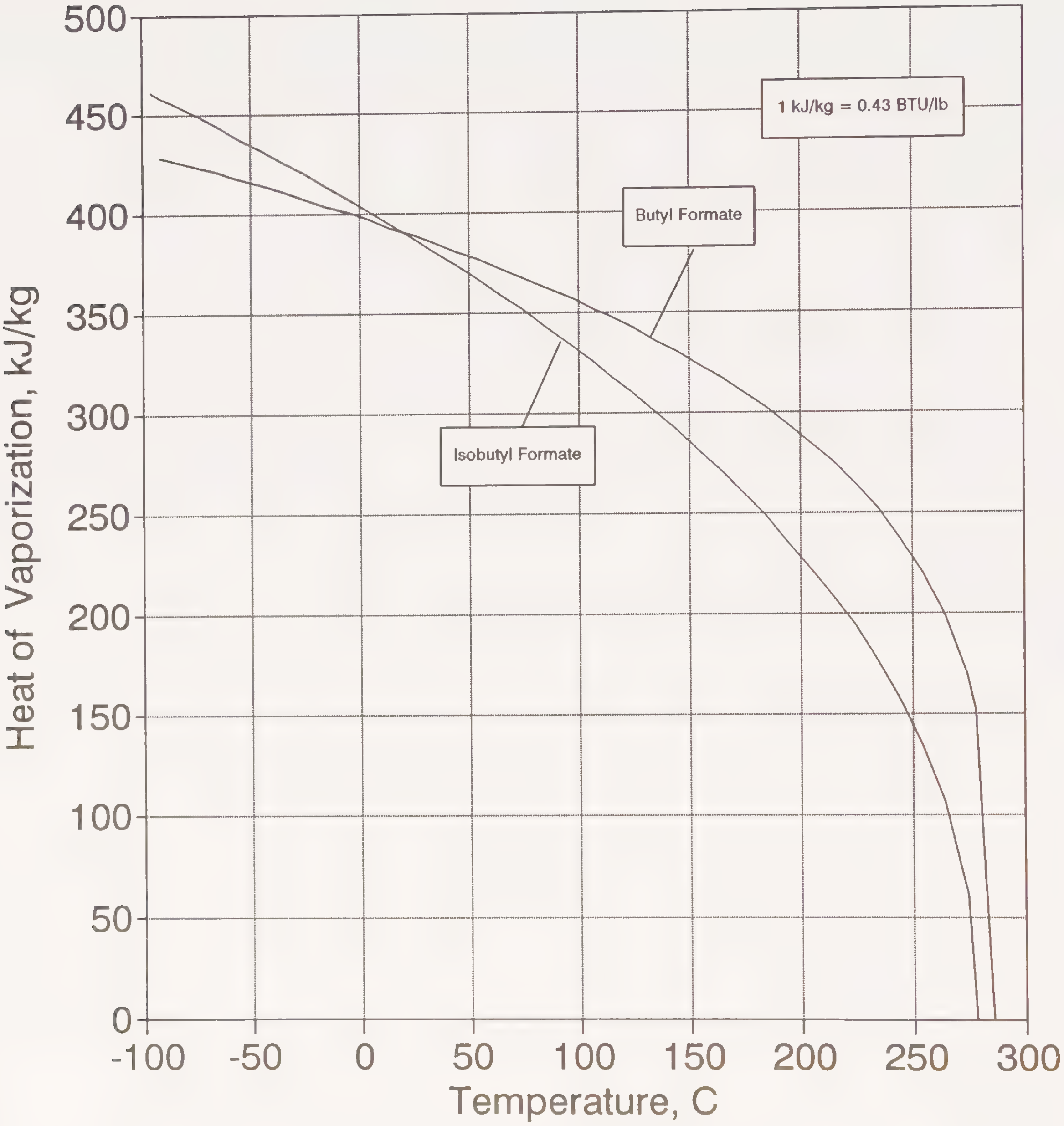

Figure 13-2 Heat of Vaporization

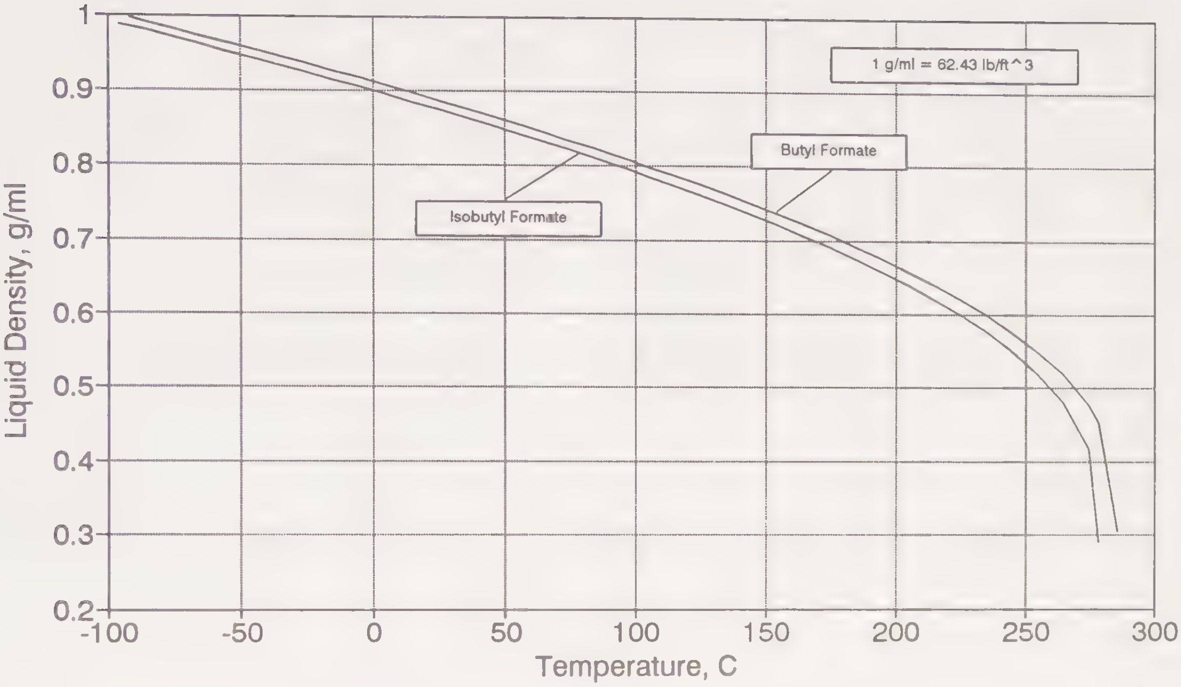

Figure 13-3 Liquid Density

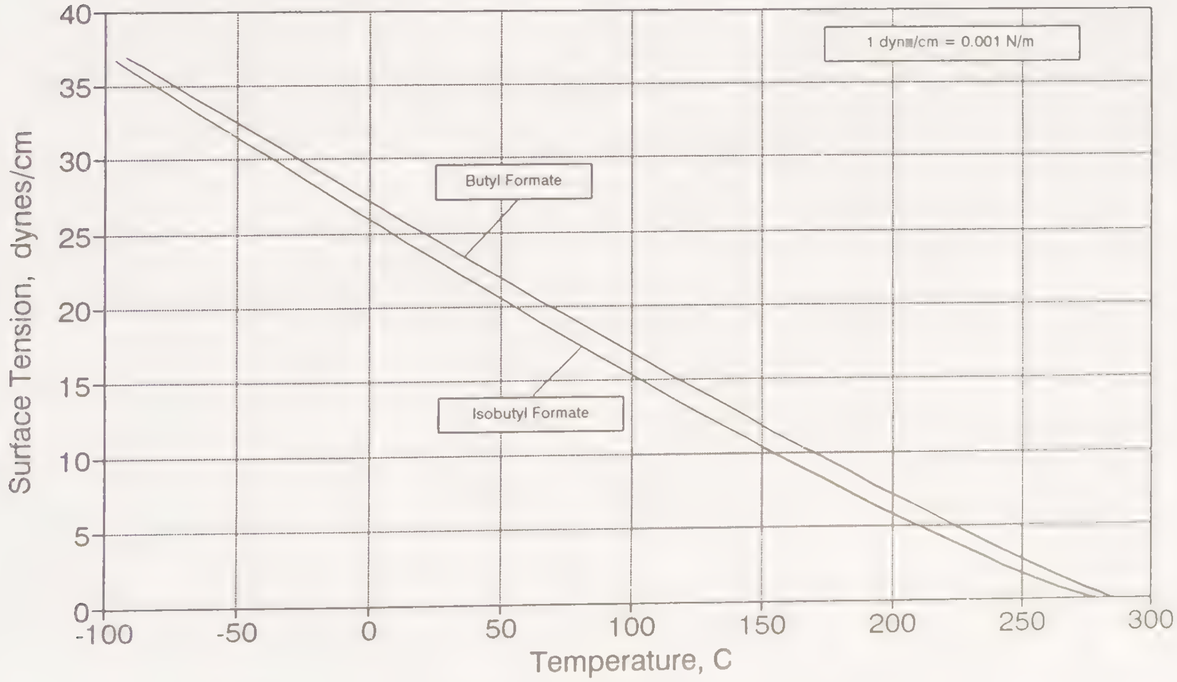

Figure 13-4 Surface Tension

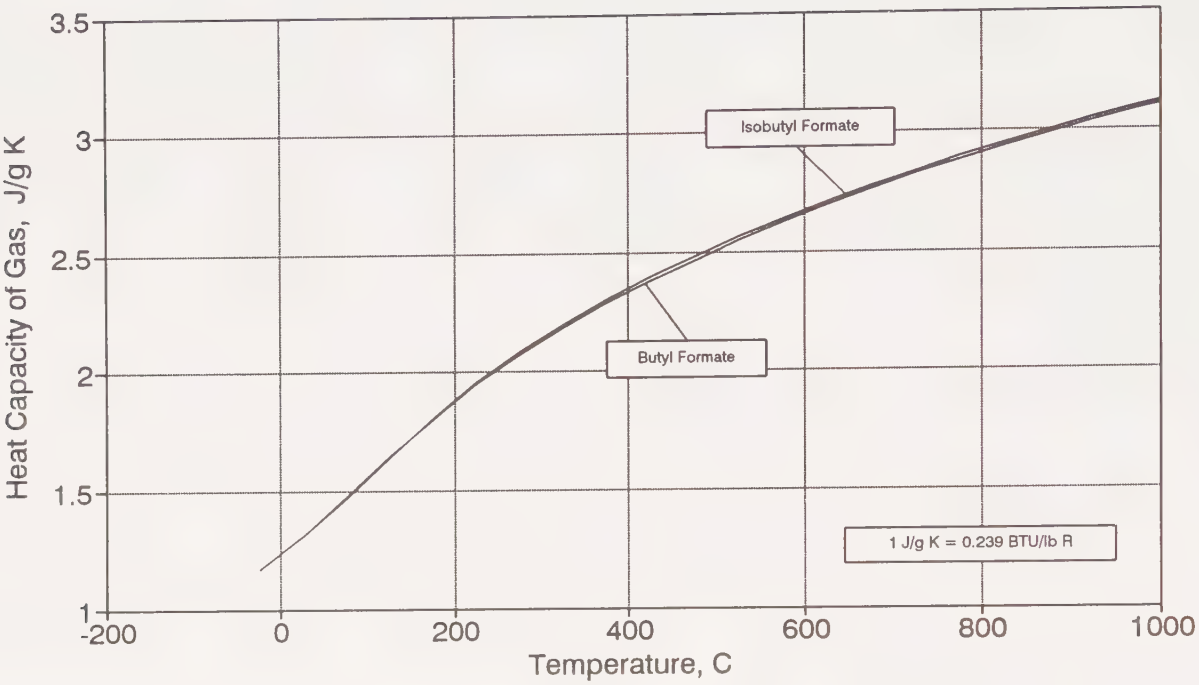

Figure 13-5 Heat Capacity of Gas

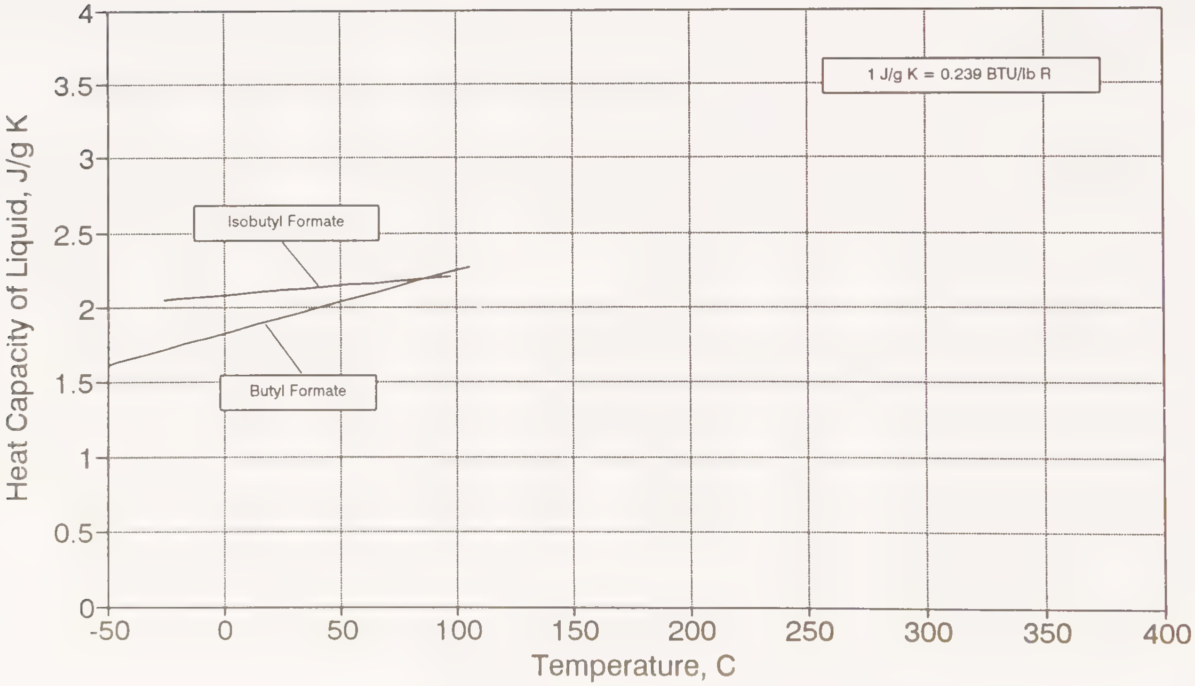

Figure 13-6 Heat Capacity of Liquid

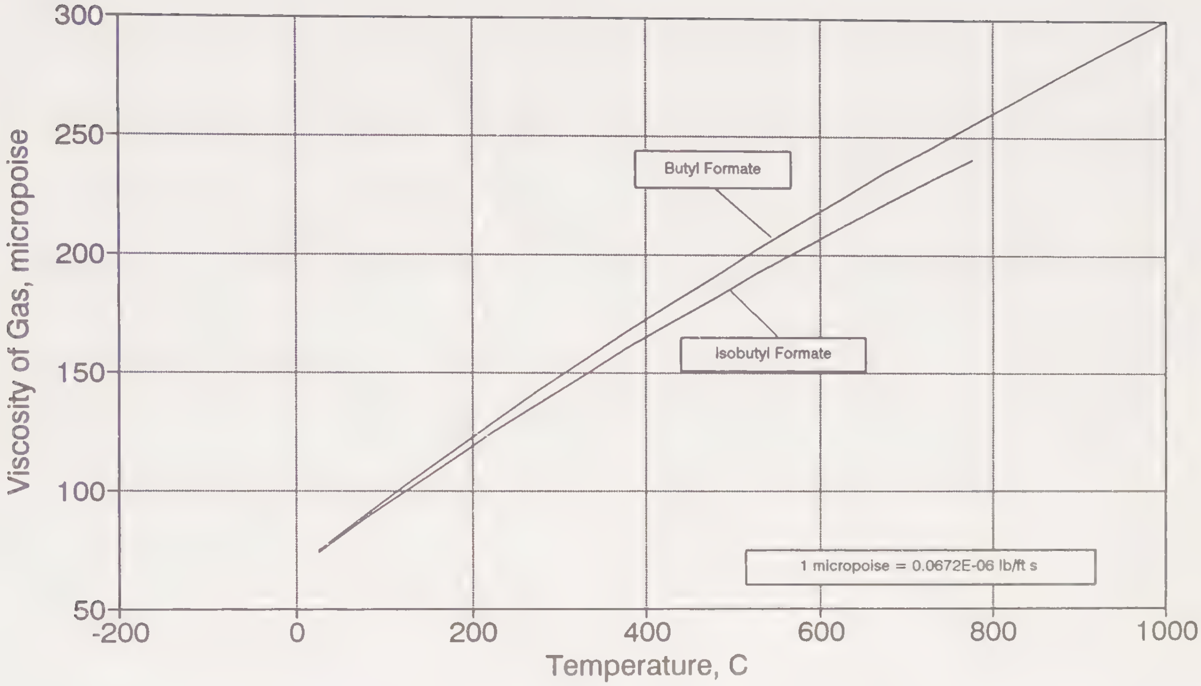

Figure 13-7 Viscosity of Gas

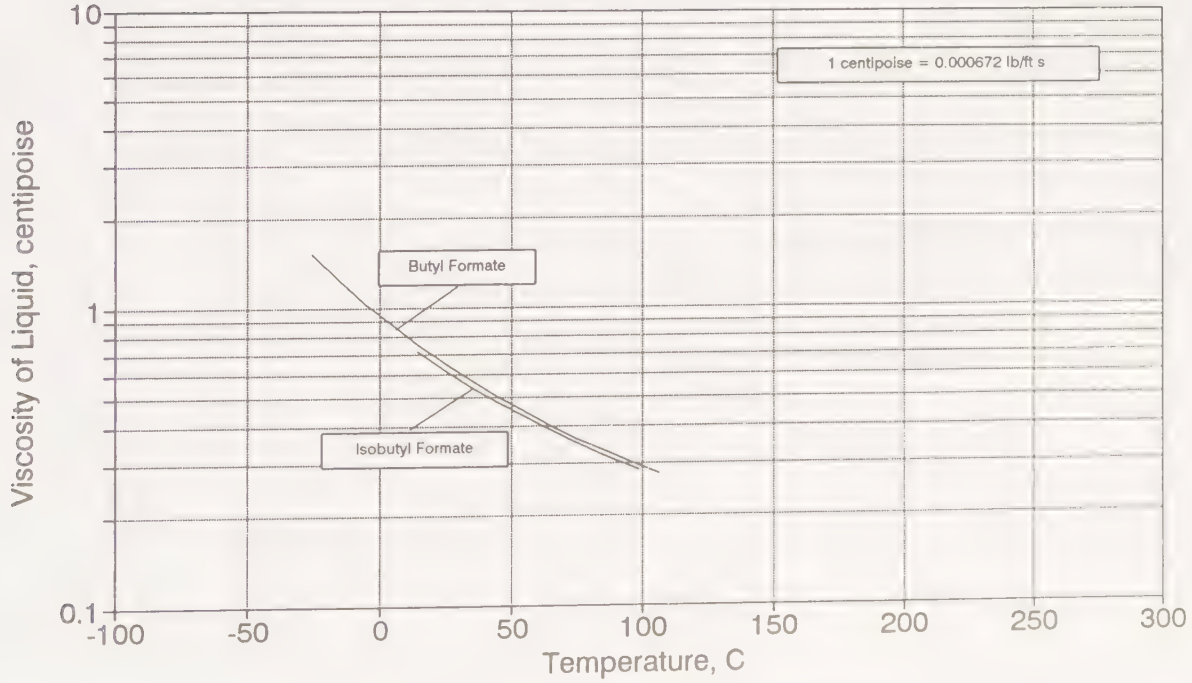

Figure 13-8 Viscosity of Liquid

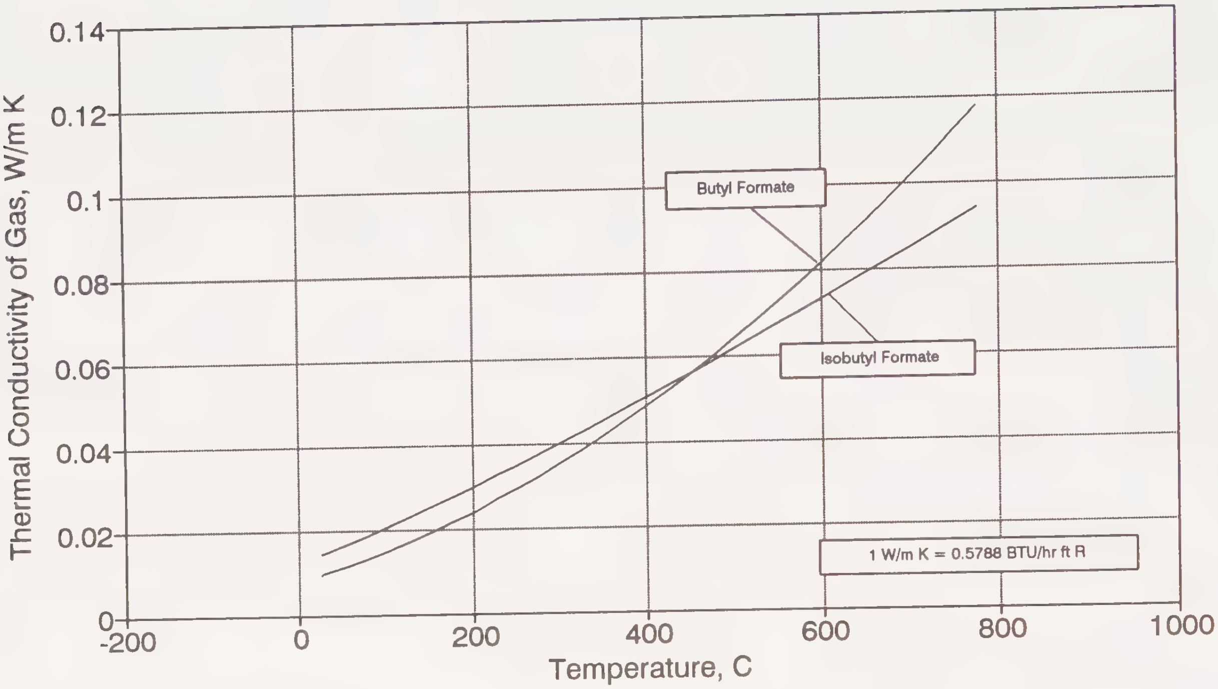

Figure 13-9 Thermal Conductivity of Gas

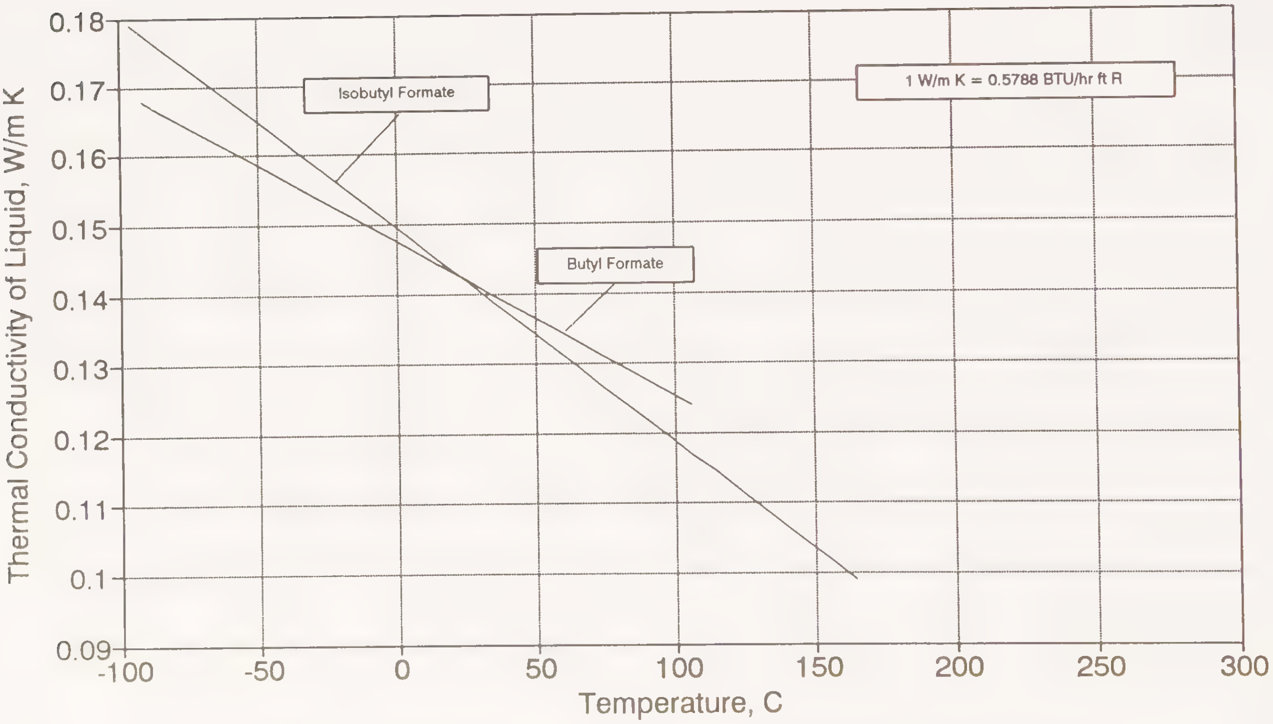

Figure 13-10 Thermal Conductivity of Liquid

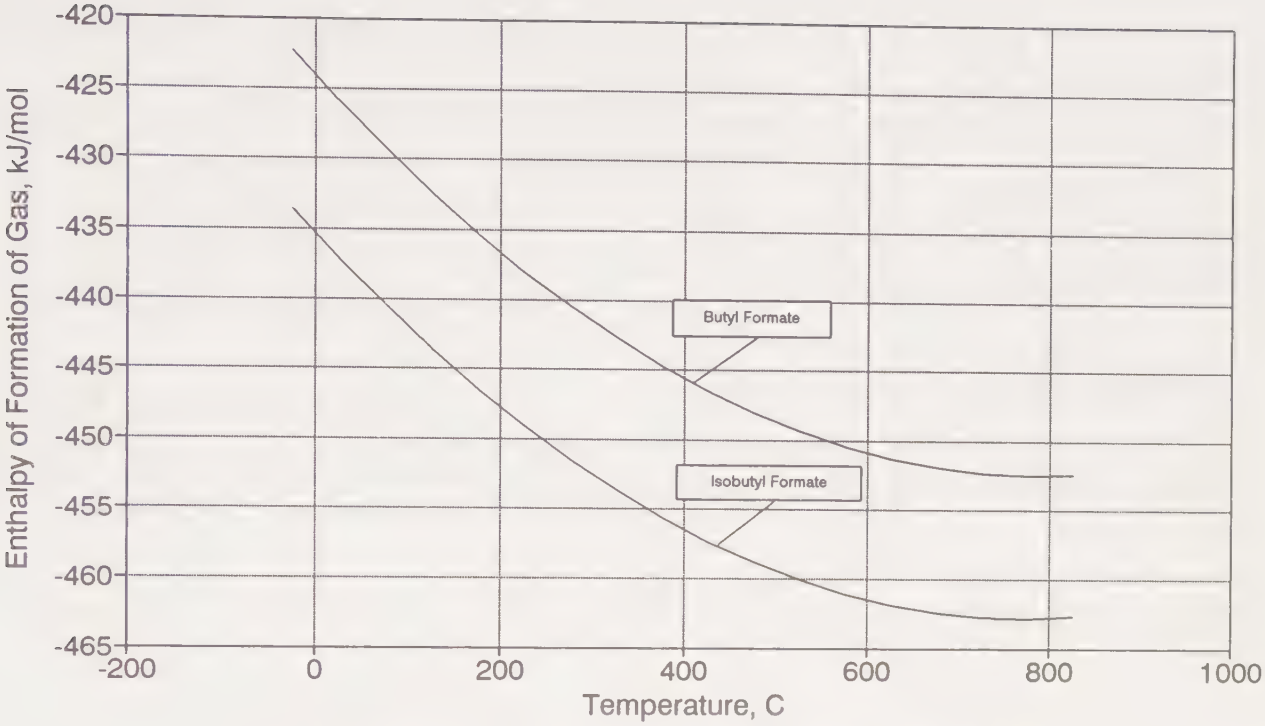

Figure 13-11 Enthalpy of Formation of Gas

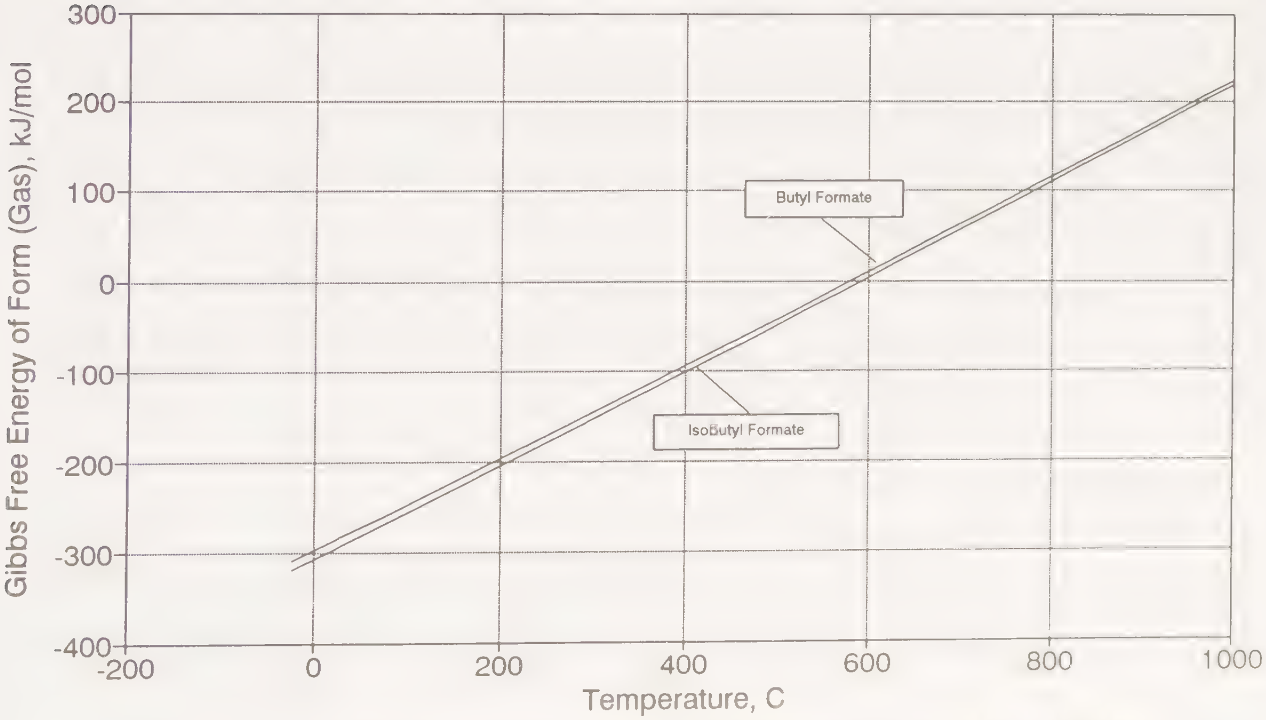

Figure 13-12 Gibbs Free Energy of Formation of Gas

Chapter 14

C_3 ACETATES

Robert W. Gallant, Carl L. Yaws and Li Bu

PHYSICAL PROPERTIES - Table 14-1

Property data from the literature (2,3,8,23,26,36,63-66,73,77,79,90,115,125,152,183-189) are given in Table 18-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available.

VAPOR PRESSURE - Figure 14-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 3% or less in most cases.

HEAT OF VAPORIZATION - Figure 14-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 3%.

LIQUID DENSITY - Figure 14-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

SURFACE TENSION - Figure 14-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 14-5 and 14-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 10% or less in most cases except for isopropyl acetate (possible 25% error).

VISCOSITY - Figures 14-7 and 14-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 10% or less in most cases except for propyl acetate (possible 25% error).

THERMAL CONDUCTIVITY - Figures 14-9 and 14-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 10% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 14-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 14-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 14-1 Physical Properties

1. Name	Isopropyl Acetate	Propyl Acetate
2. Formula	C5H10O2	C5H10O2
3. Molecular Weight, g/mol	102.133	102.133
4. Critical Temperature, K	538.00	549.40
5. Critical Pressure, bar	35.800	33.600
6. Critical Volume, ml/mol	336.00	345.00
7. Critical Compressibility Factor	0.269	0.254
8. Acentric Factor	0.3550	0.3935
9. Melting Point, K	199.75	178.15
10. Boiling Point @ 1 atm, K	361.65	374.65
11. Heat of Vaporization @ BP, kJ/kg	315.55	337.51
12. Density of Liquid @ 25 C, g/ml	0.871	0.883
13. Surface Tension @ 25 C, dynes/cm	21.280	23.863
14. Heat Capacity of Gas @ 25 C, J/g K	1.286	1.331
15. Heat Capacity of Liquid @ 25 C, J/g K	1.953	1.921
16. Viscosity of Gas @ 25 C, micropoise	69.696	67.903
17. Viscosity of Liquid @ 25 C, centipoise	0.531	0.551
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.011	0.010
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.135	0.141
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-482.49	-465.48
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-334.881	-321.610
22. Flash Point, K	275.37	288.00
23. Autoignition Temperature, K	752.15	723.00
24. Lower Explosion Limit in Air, vol %	1.8	2.0
25. Upper Explosion Limit in Air, vol %	7.2	8.0
26. Solubility in Water @ 25 C, ppm(wt)	------	------

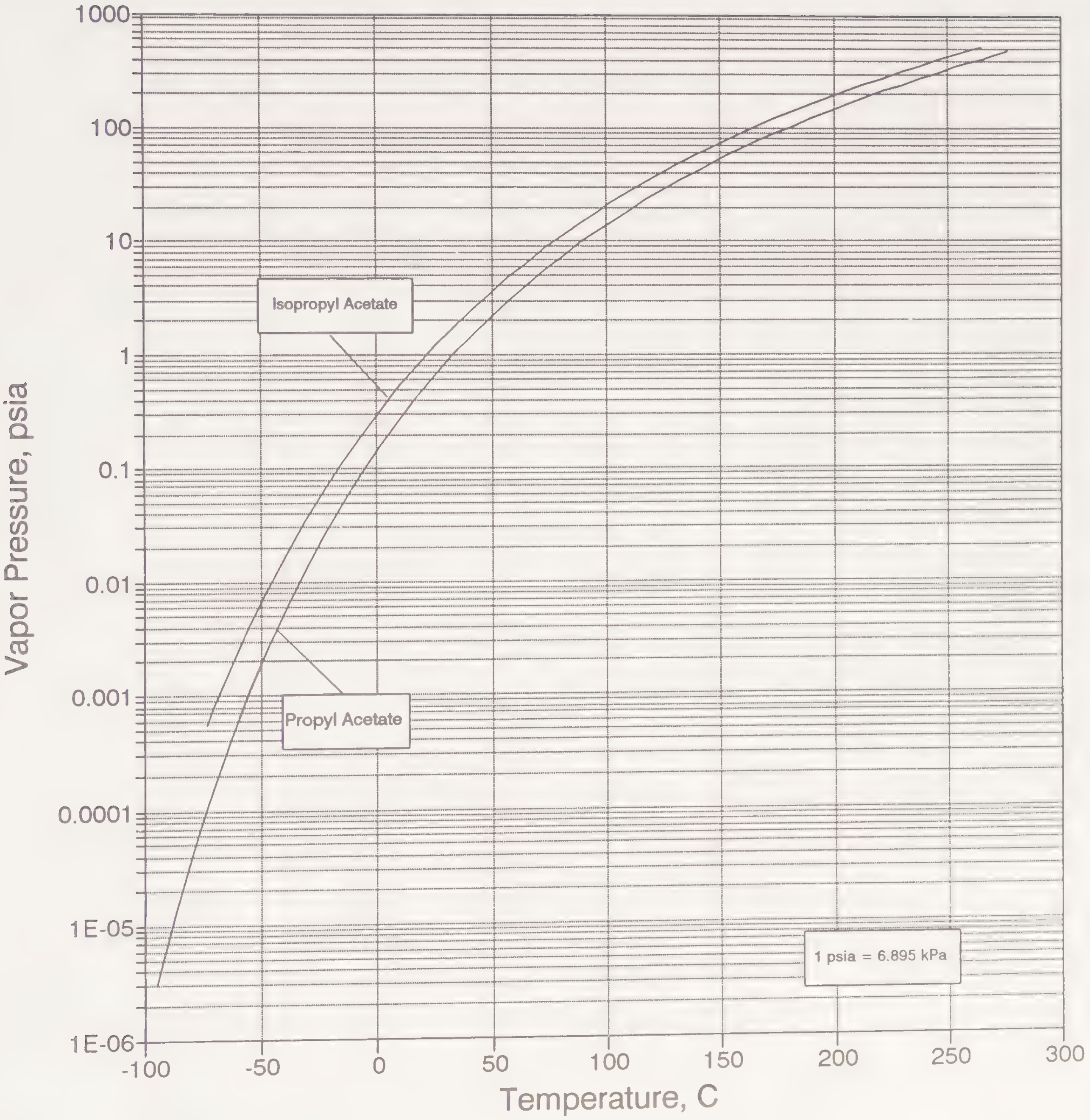

Figure 14-1 Vapor Pressure

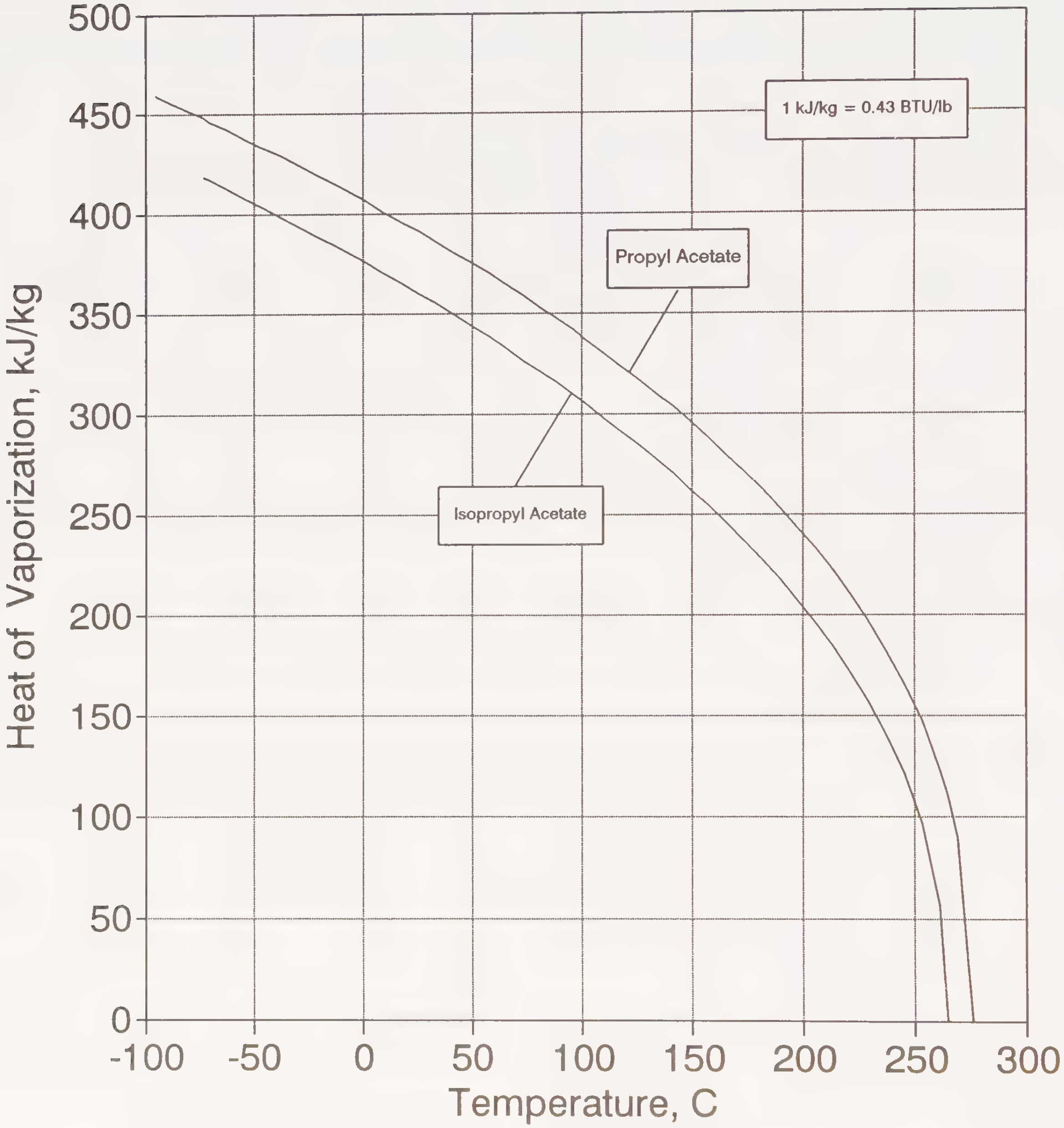

Figure 14-2 Heat of Vaporization

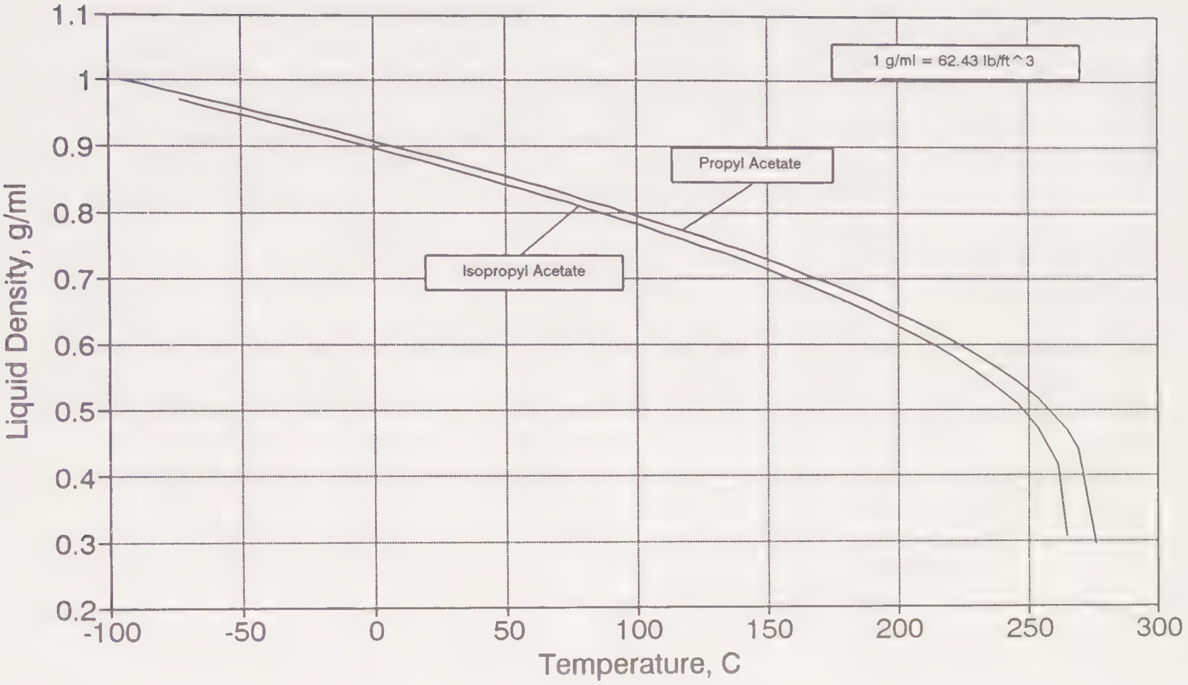

Figure 14-3 Liquid Density

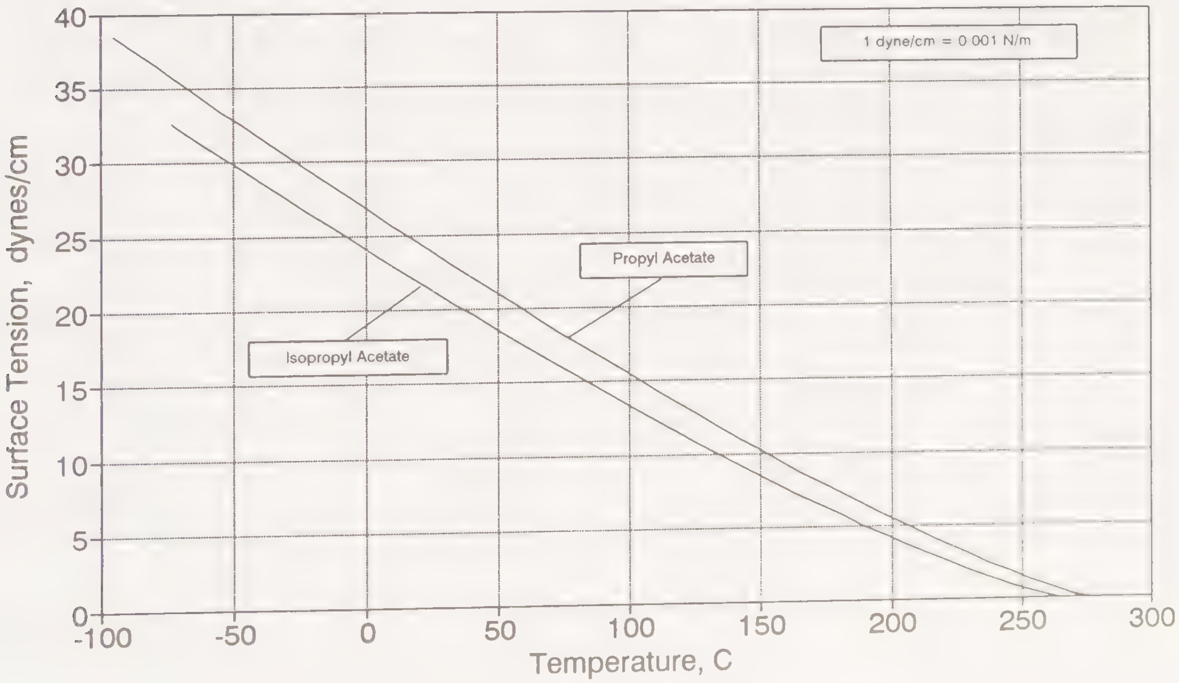

Figure 14-4 Surface Tension

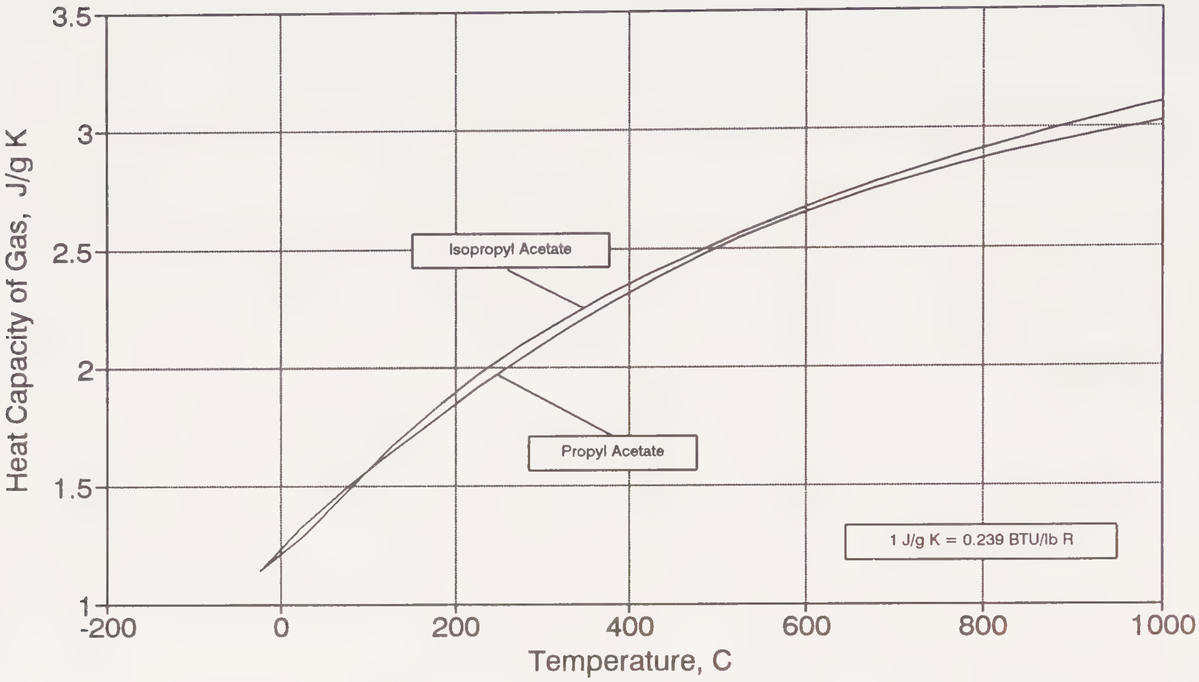

Figure 14-5 Heat Capacity of Gas

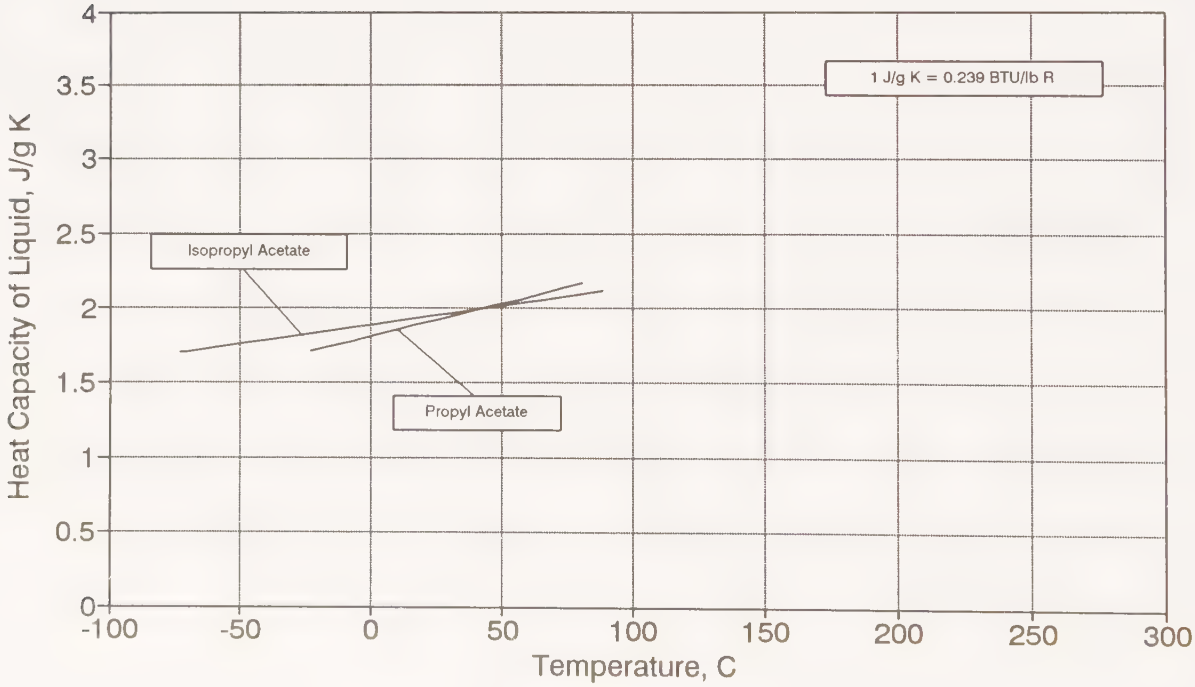

Figure 14-6 Heat Capacity of Liquid

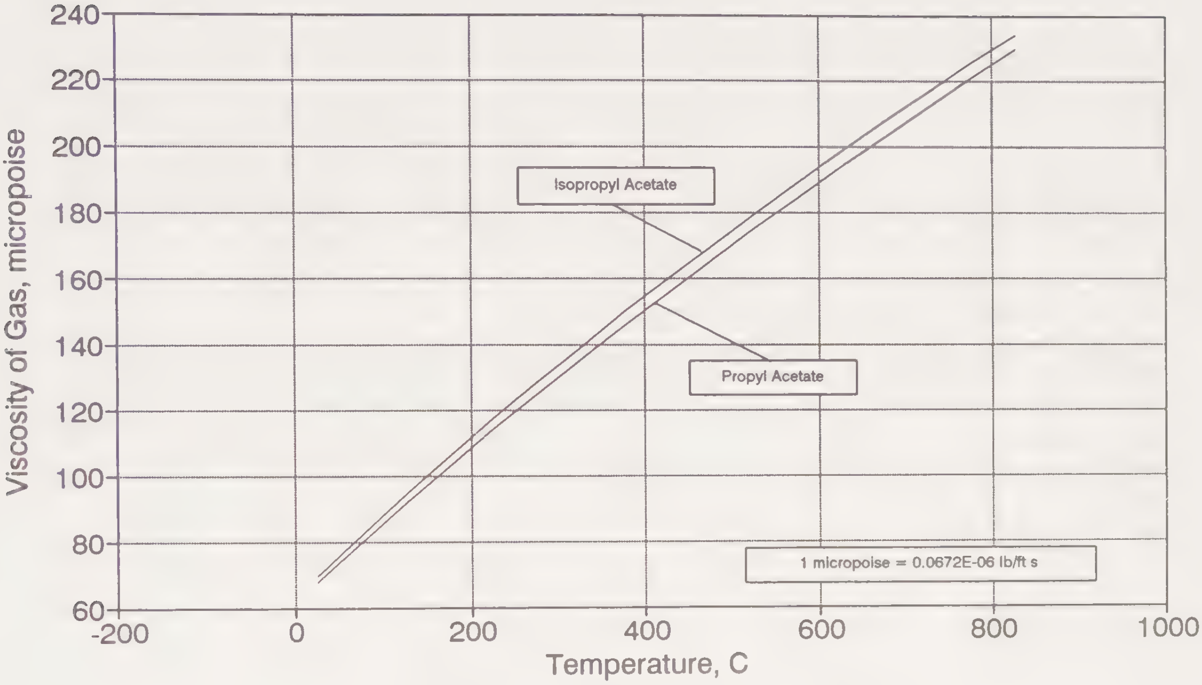

Figure 14-7 Viscosity of Gas

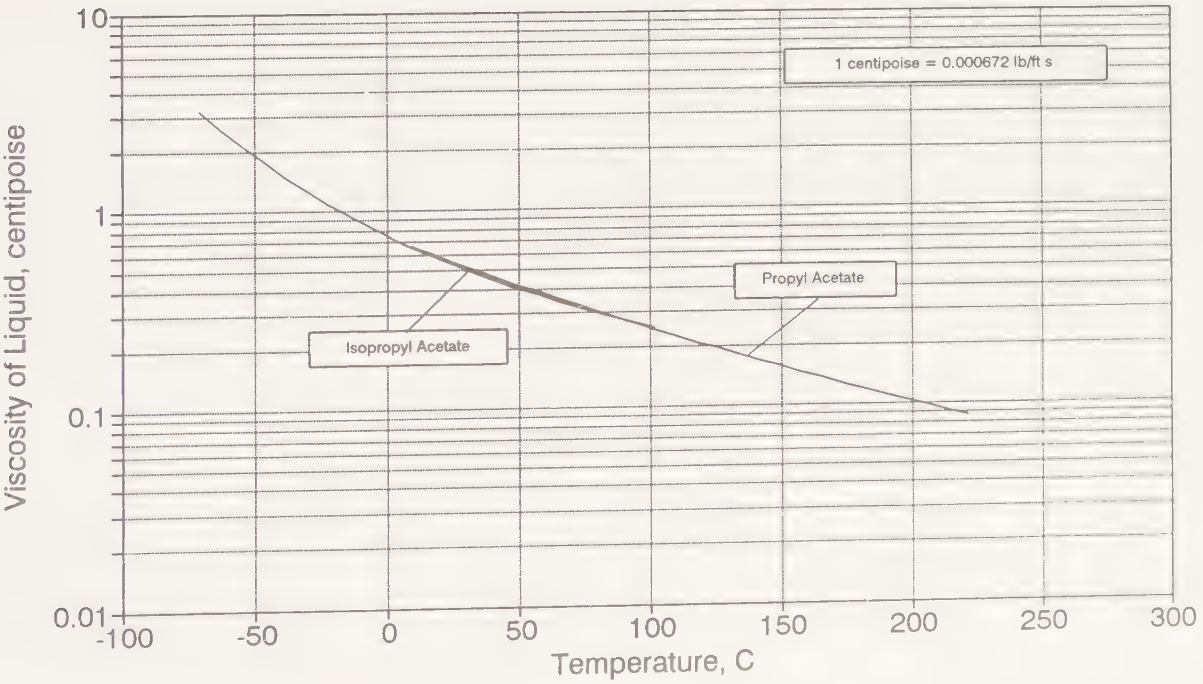

Figure 14-8 Viscosity of Liquid

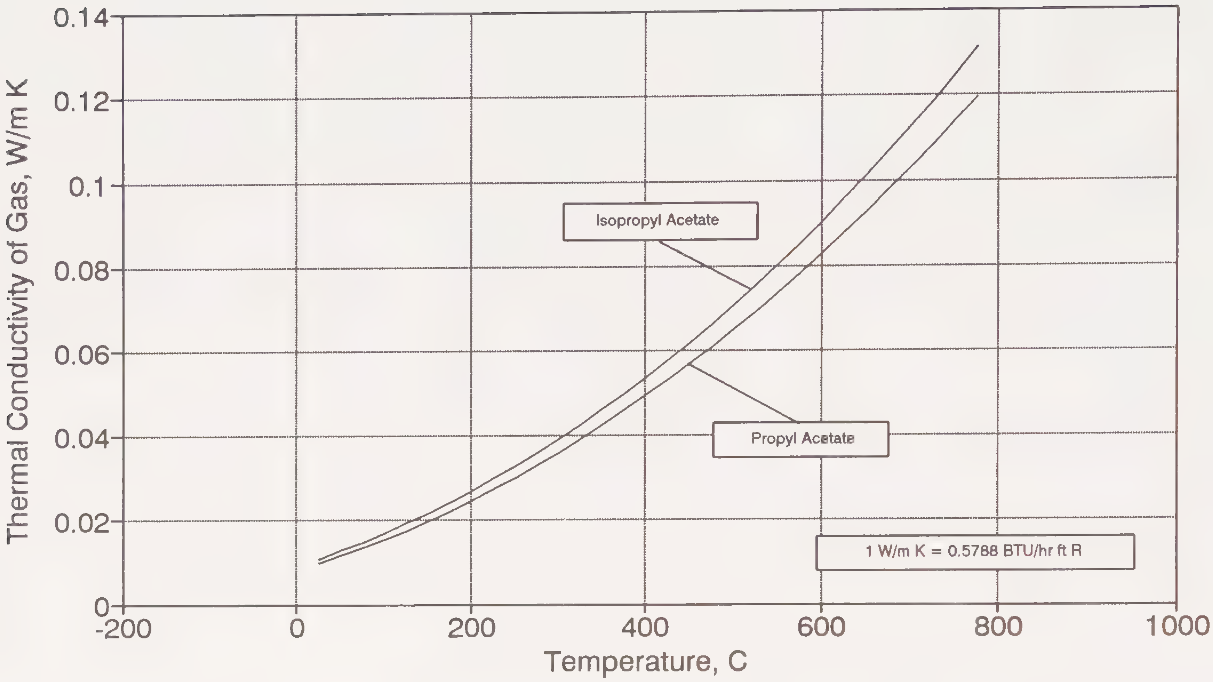

Figure 14-9 Thermal Conductivity of Gas

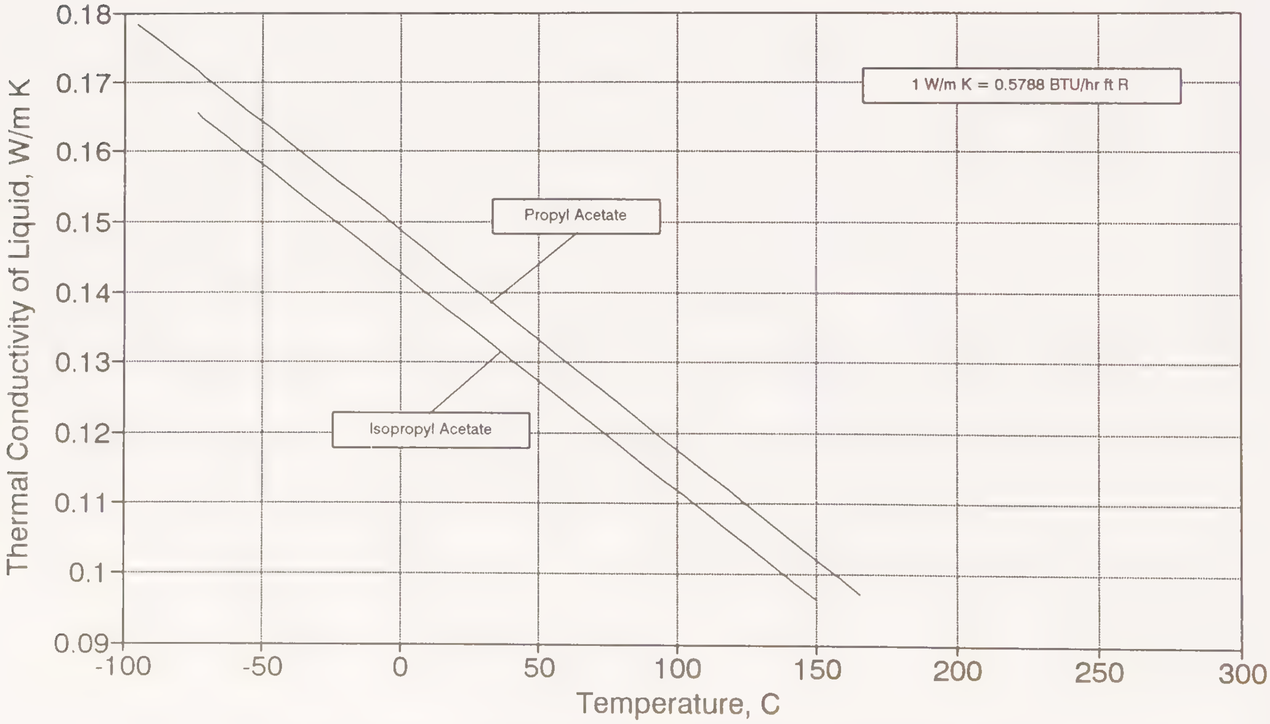

Figure 14-10 Thermal Conductivity of Liquid

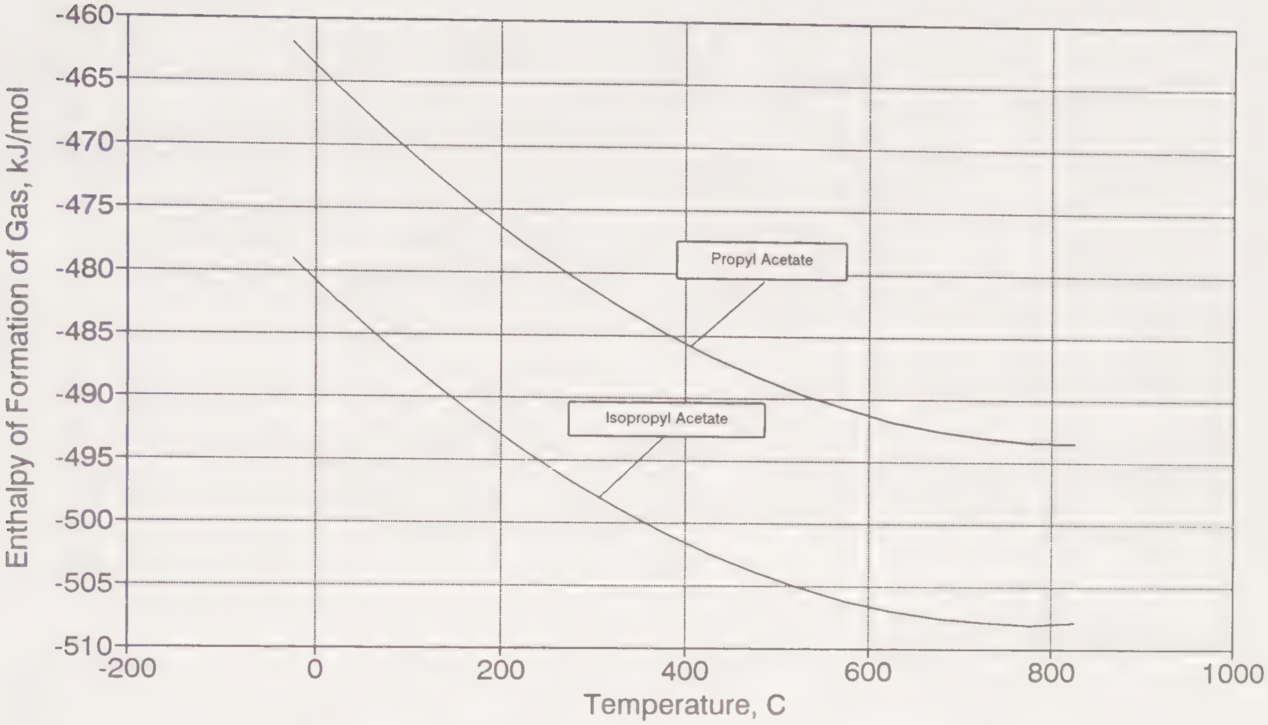

Figure 14-11 Enthalpy of Formation of Gas

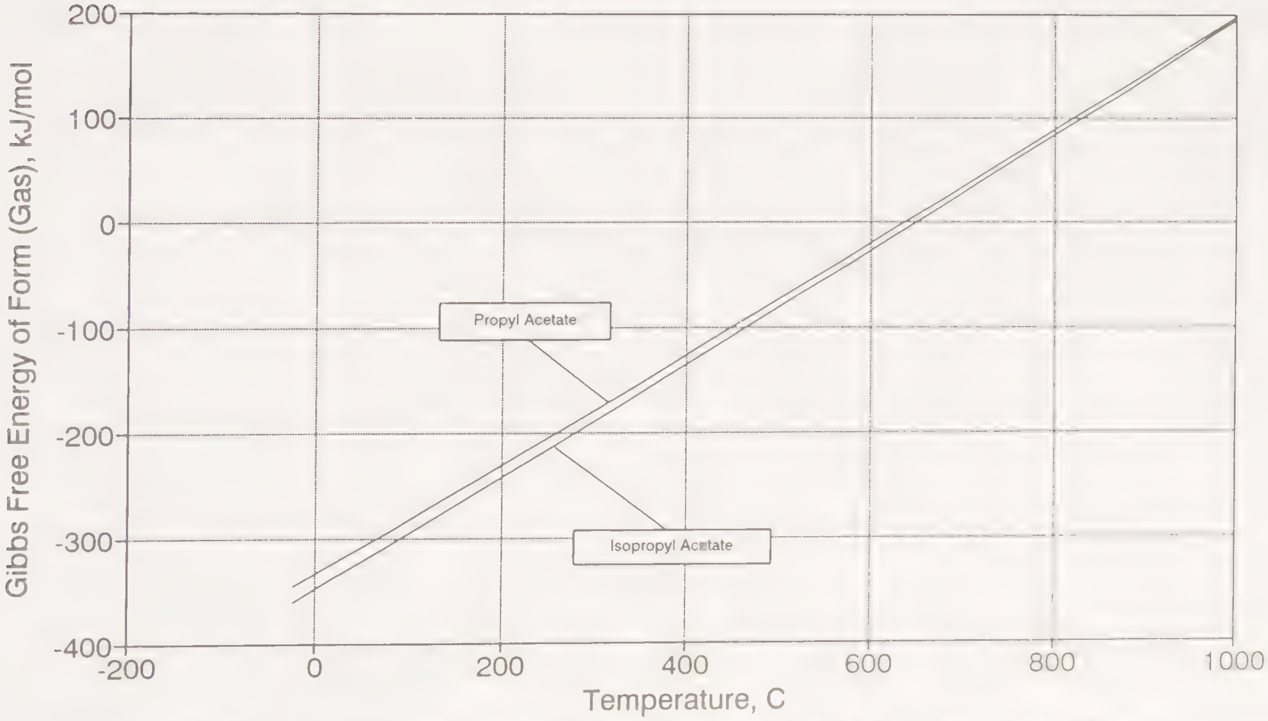

Figure 14-12 Gibbs Free Energy of Formation of Gas

Chapter 15

C_4 ACETATES

Robert W. Gallant, Carl L. Yaws and Li Bu

PHYSICAL PROPERTIES - Table 15-1

Property data from the literature (8,20,25,63-65,68,73,75,77,79,82,87,90,95,103,109,121,123,125,155,180,184-186,199-207) are given in Table 15-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available.

VAPOR PRESSURE - Figure 15-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 10% or less in most cases.

HEAT OF VAPORIZATION - Figure 15-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 10%.

LIQUID DENSITY - Figure 15-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

SURFACE TENSION - Figure 15-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 15-5 and 15-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 5% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 25% or less in most cases.

VISCOSITY - Figures 15-7 and 15-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 10% or less in most cases except for tert-Butyl Acetate (possible 25% error).

THERMAL CONDUCTIVITY - Figures 15-9 and 15-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most casesexcept for methyl sec-butyl ether (possible 25% error).

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 15-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 15-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 15-1 Physical Properties

1. Name	Butyl Acetate	sec-Butyl Acetate	tert-Butyl Acetate
2. Formula	C6H12O2	C6H12O2	C6H12O2
3. Molecular Weight, g/mol	116.160	116.160	116.160
4. Critical Temperature, K	579.15	561.00	545.00
5. Critical Pressure, bar	31.100	31.700	31.700
6. Critical Volume, ml/mol	389.00	389.00	389.00
7. Critical Compressibility Factor	0.251	0.264	0.272
8. Acentric Factor	0.4101	0.4056	0.3431
9. Melting Point, K	199.65	174.15	------
10. Boiling Point @ 1 atm, K	399.15	385.15	369.15
11. Heat of Vaporization @ BP, kJ/kg	314.08	298.58	280.45
12. Density of Liquid @ 25 C, g/ml	0.876	0.868	0.861
13. Surface Tension @ 25 C, dynes/cm	24.75	23.06	21.56
14. Heat Capacity of Gas @ 25 C, J/g K	1.38	1.34	1.34
15. Heat Capacity of Liquid @ 25 C, J/g K	1.96	1.98	1.99
16. Viscosity of Gas @ 25 C, micropoise	63.18	64.94	67.56
17. Viscosity of Liquid @ 25 C, centipoise	0.687	0.656	0.569
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.010	0.013	0.011
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.135	0.131	0.123
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-486.51	-504.75	-524.01
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-313.71	-331.20	-340.37
22. Flash Point, K	295.00	288.71	289.00
23. Autoignition Temperture, K	694.00	695.00	------
24. Lower Explosion Limit in Air, vol %	1.7	1.7	1.3
25. Upper Explosion Limit in Air, vol %	7.6	7.6	7.3
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

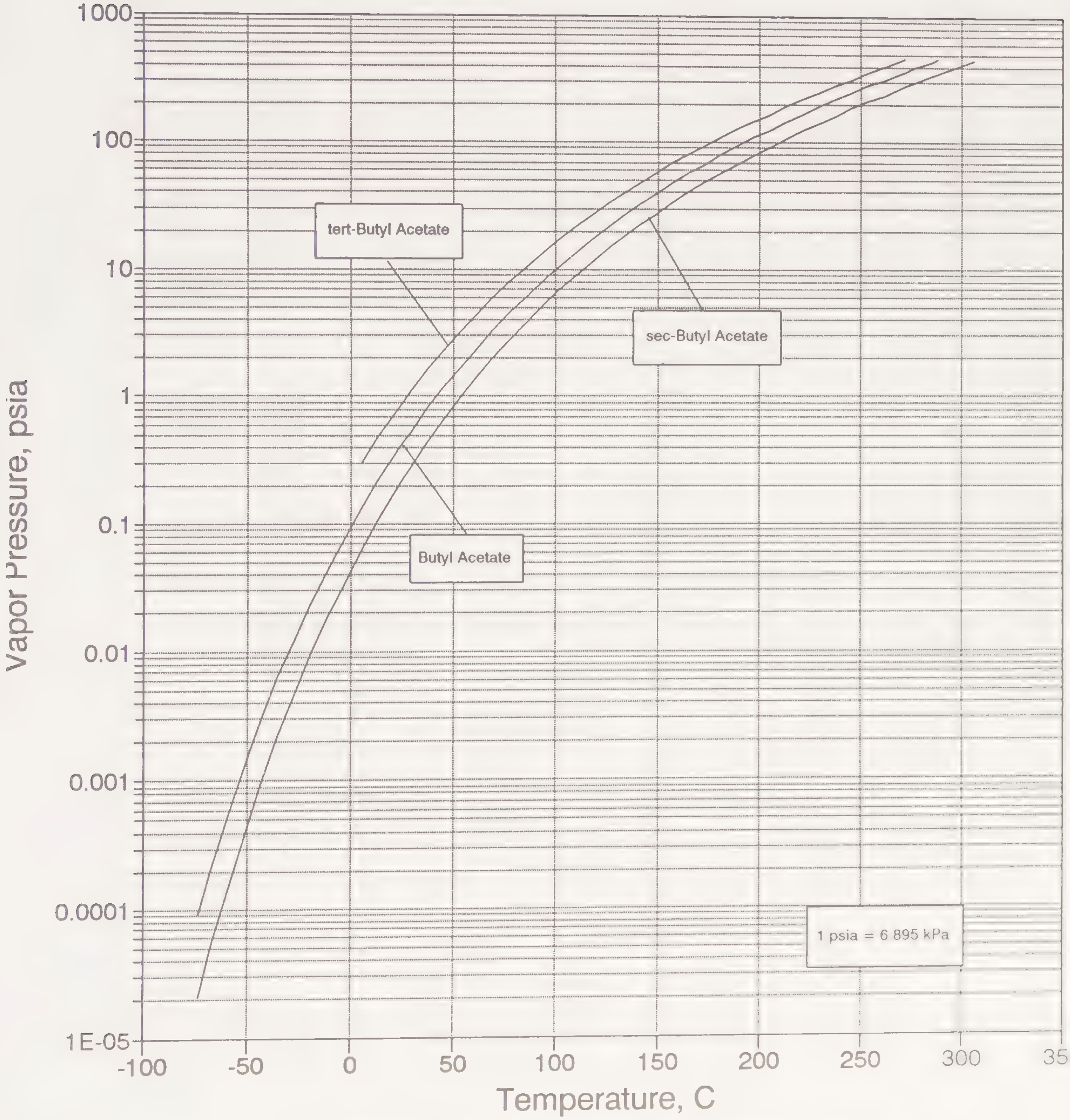

Figure 15-1 Vapor Pressure

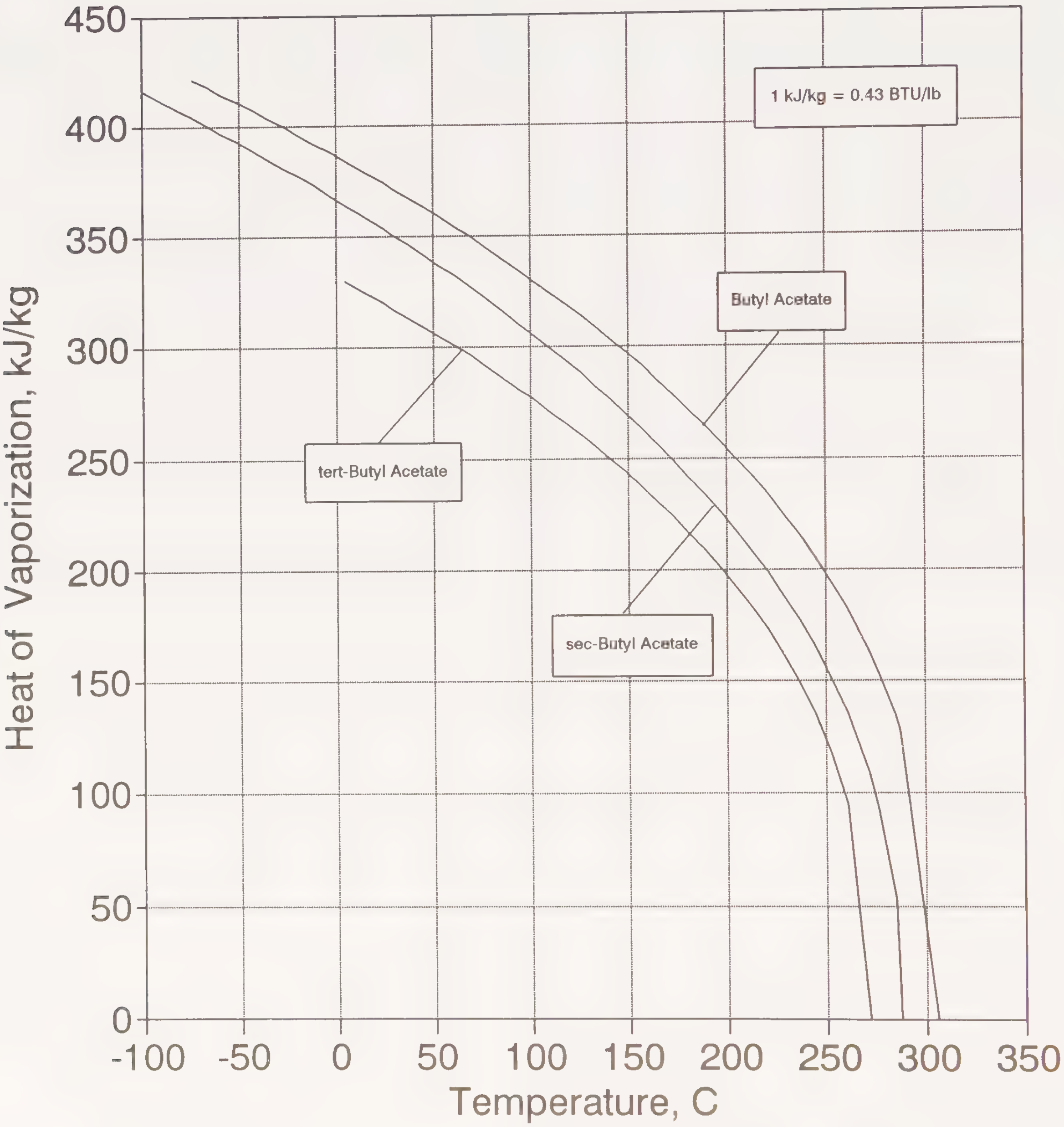

Figure 15-2 Heat of Vaporization

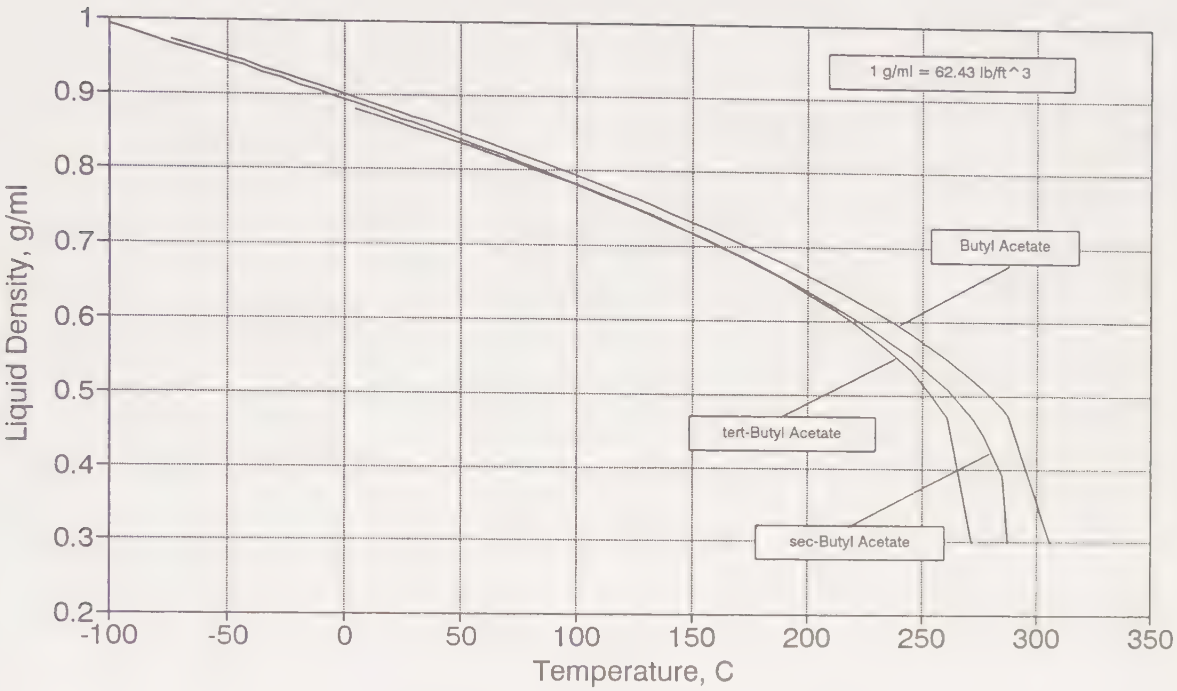

Figure 15-3 Liquid Density

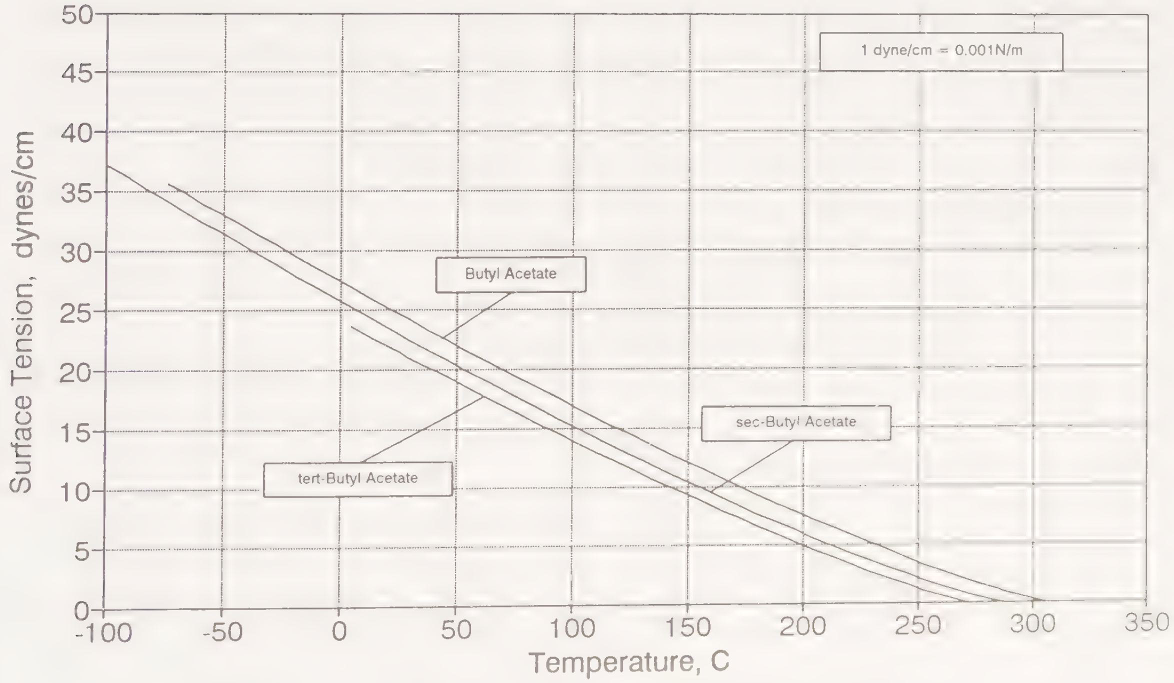

Figure 15-4 Surface Tension

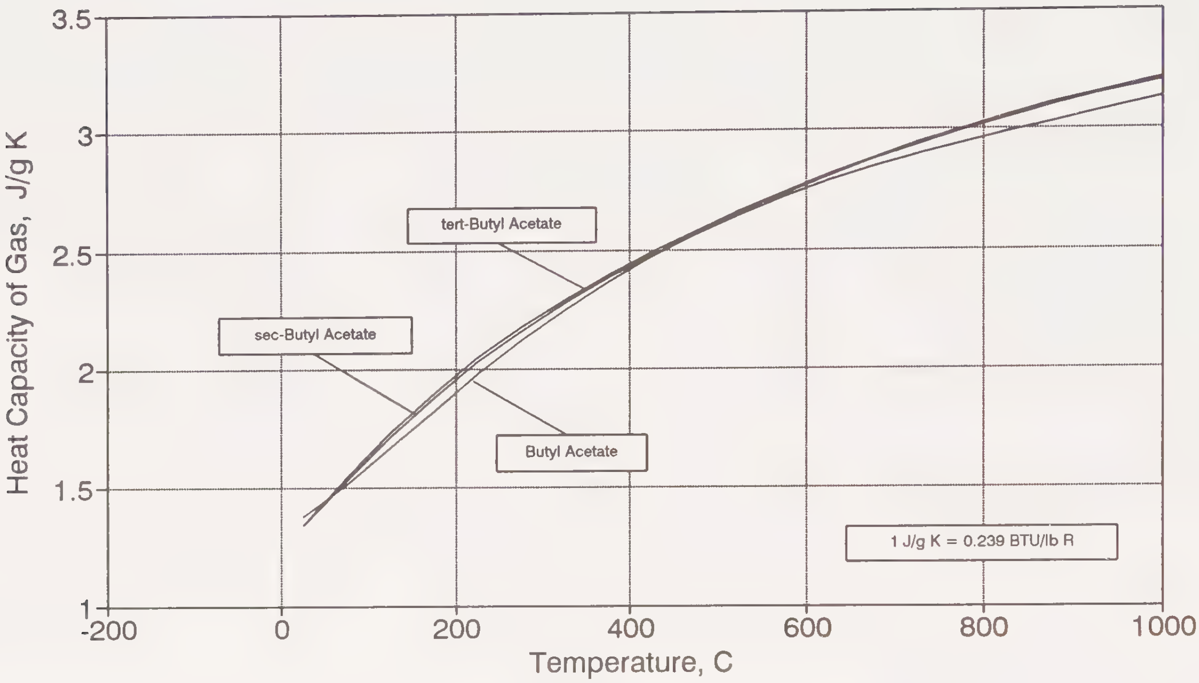

Figure 15-5 Heat Capacity of Gas

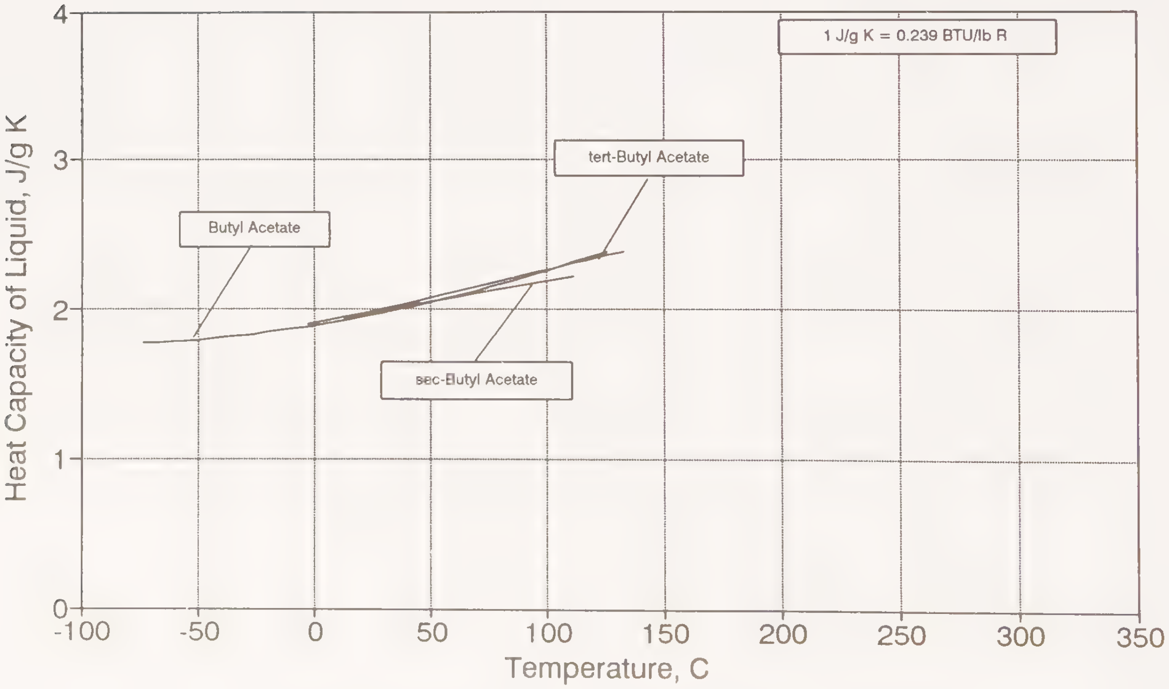

Figure 15-6 Heat Capacity of Liquid

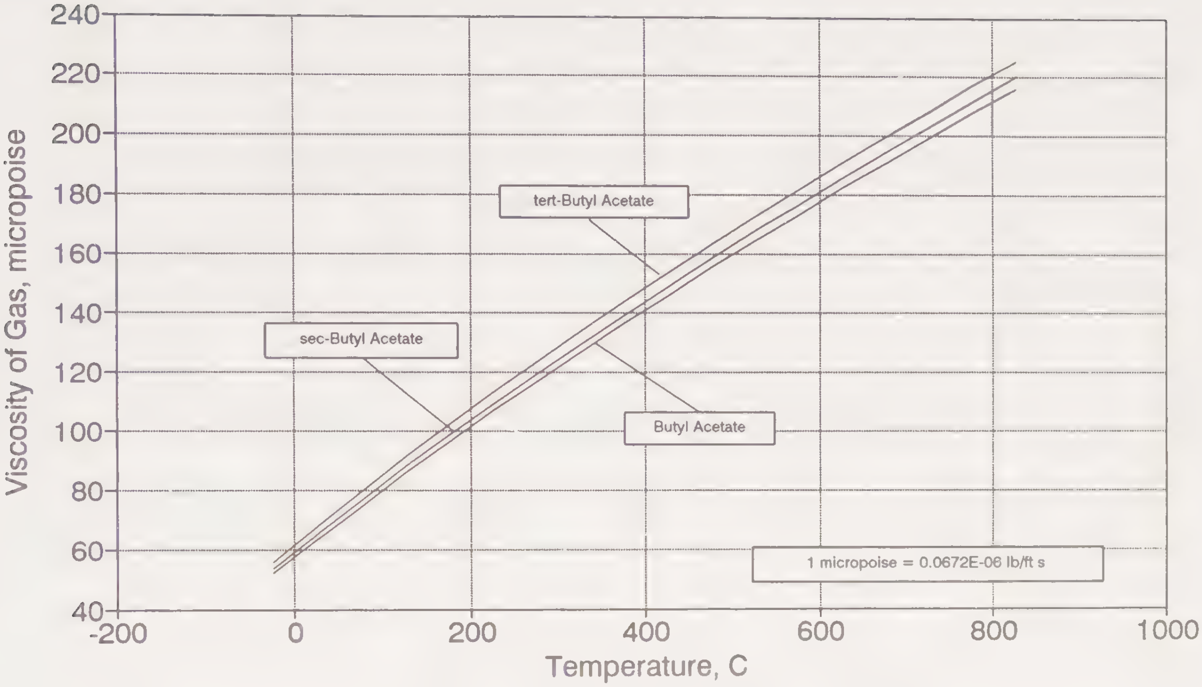

Figure 15-7 Viscosity of Gas

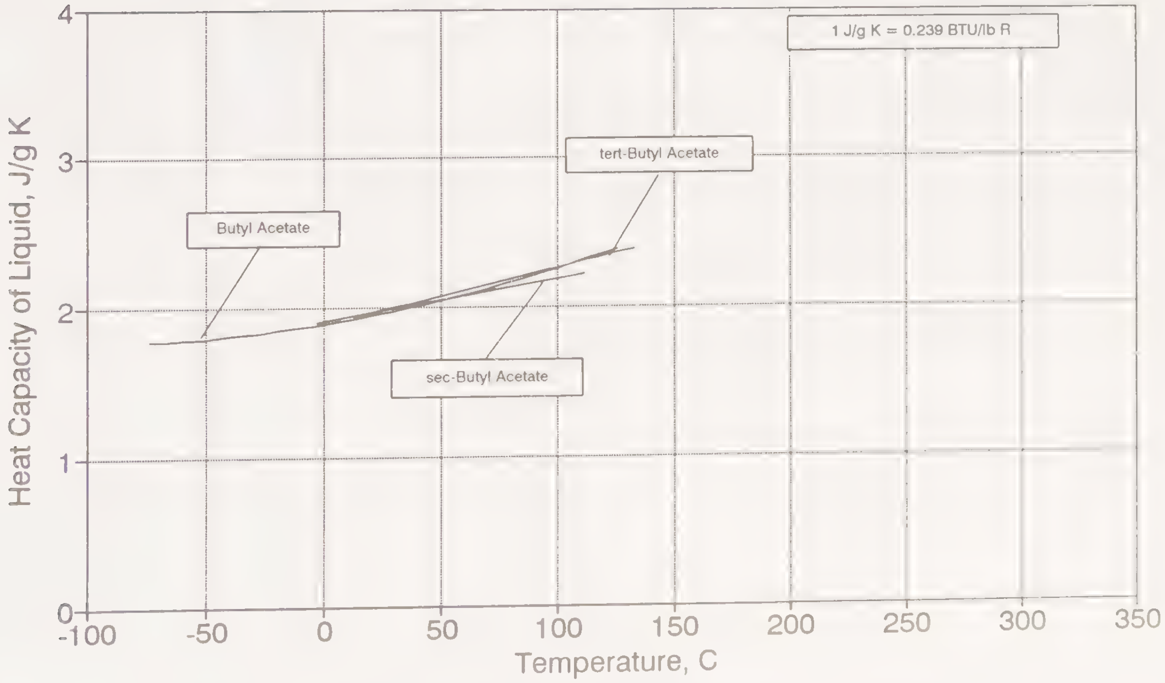

Figure 15-6 Heat Capacity of Liquid

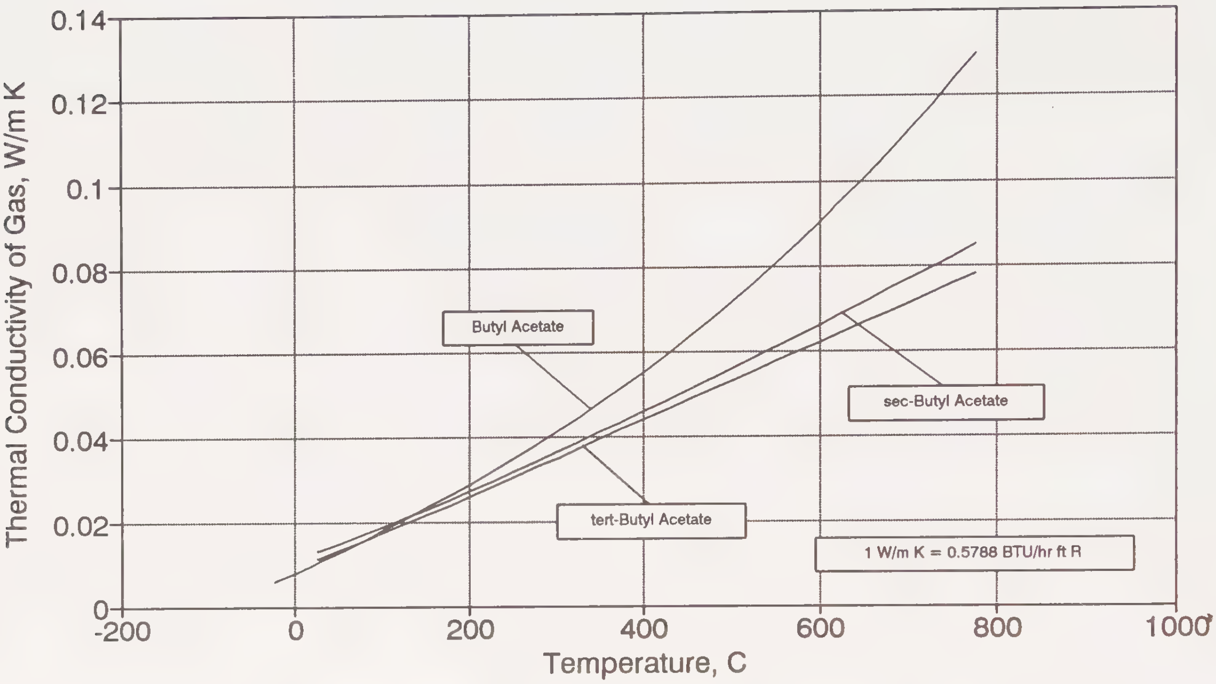

Figure 15-9 Thermal Conductivity of Gas

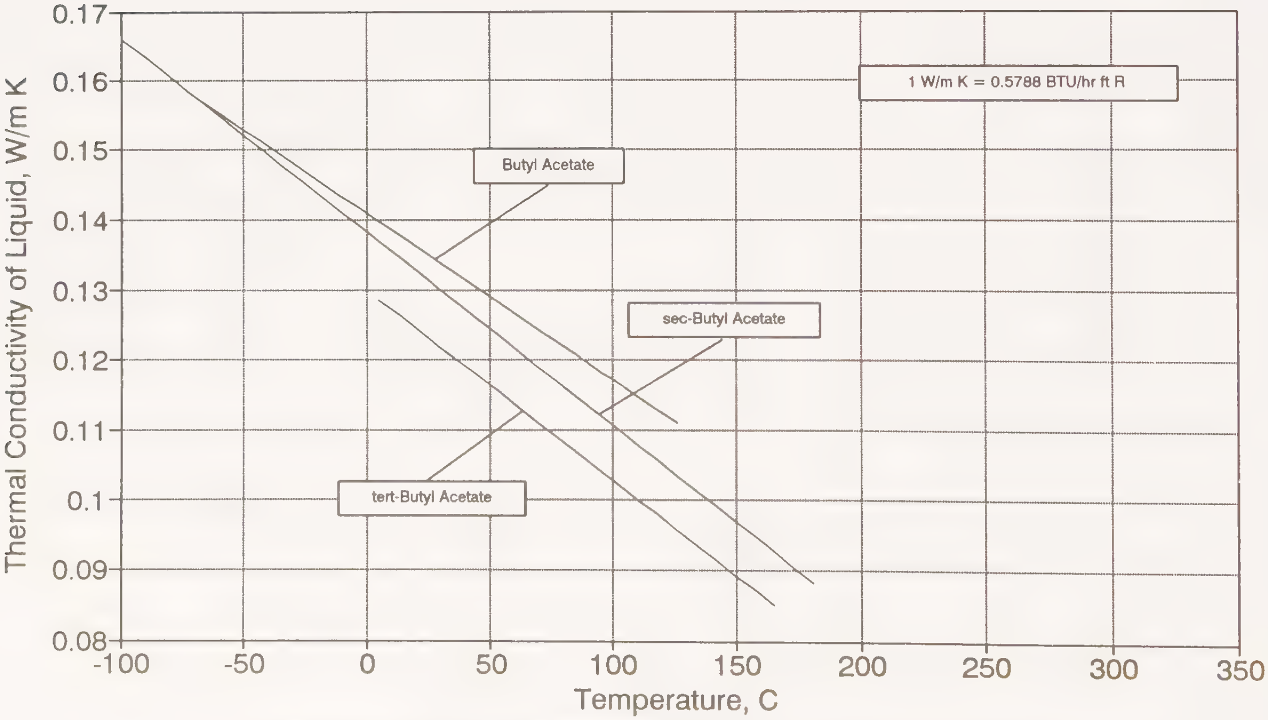

Figure 15-10 Thermal Conductivity of Liquid

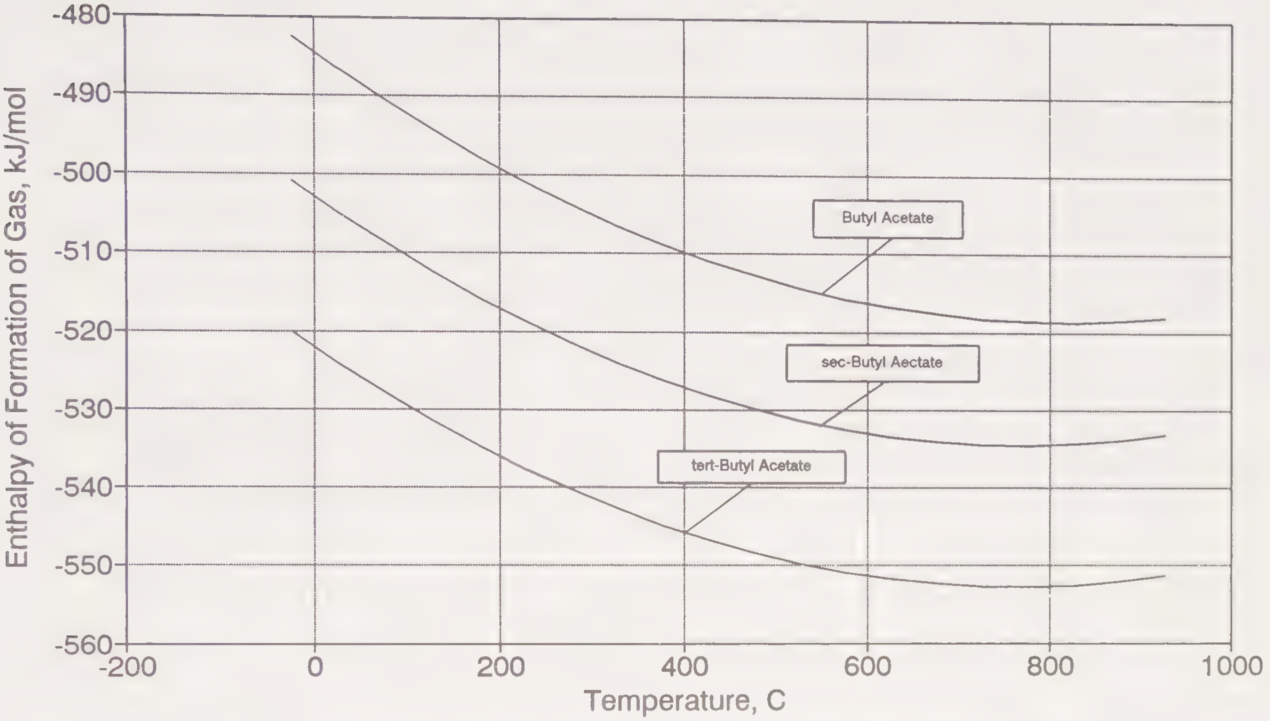

Figure 15-11 Enthalpy of Formation of Gas

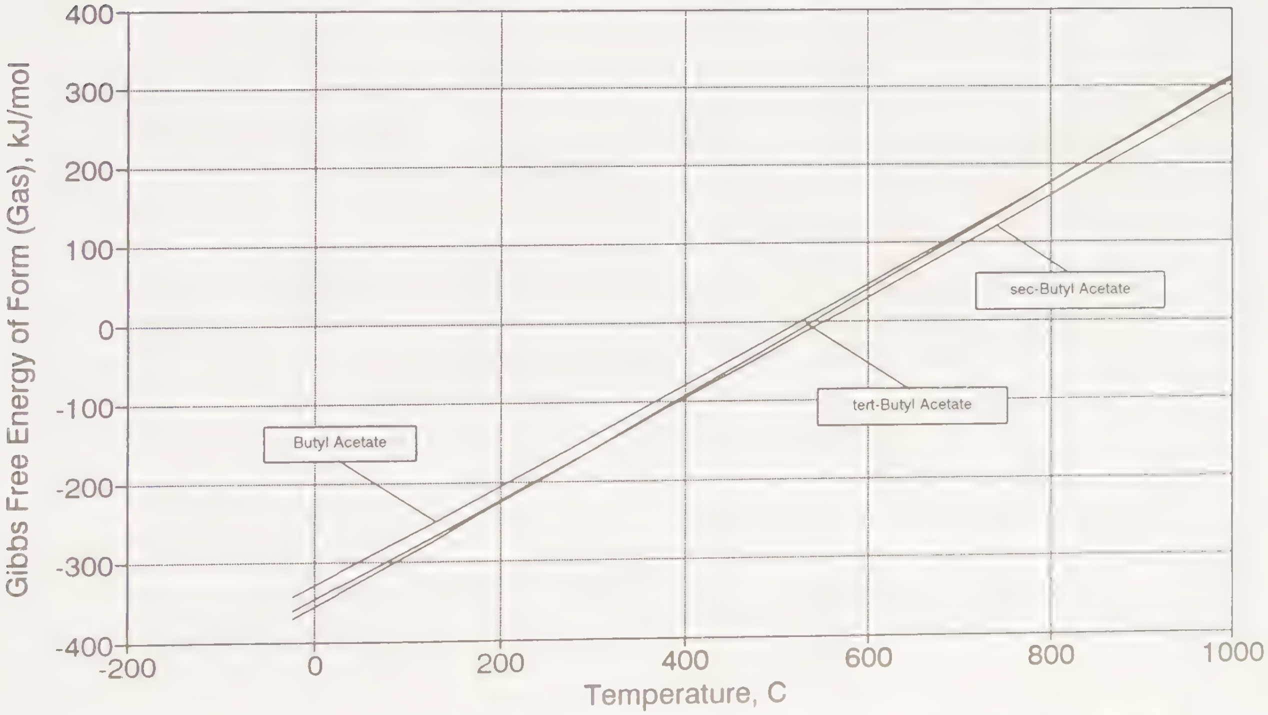

Figure 15-12 Gibbs Free Energy of Formation of Gas

Chapter 16

C_4 GLYCOLS

Robert W. Gallant, Carl L. Yaws and Li Bu

PHYSICAL PROPERTIES - Table 16-1

Property data from the literature (2,3,26,62-66,75,77,79,83,87,90,121,157,190-198) are given in Table 18-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available.

VAPOR PRESSURE - Figure 16-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 10% or less in most cases.

HEAT OF VAPORIZATION - Figure 16-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 10%.

LIQUID DENSITY - Figure 16-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 5% in most cases.

SURFACE TENSION - Figure 16-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 10% or less in most cases.

HEAT CAPACITY - Figures 16-5 and 16-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 5% or less in most cases except for 1,3 butylene glycol (possible 25% error).

VISCOSITY - Figures 16-7 and 16-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 10% or less in most cases.

THERMAL CONDUCTIVITY - Figures 16-9 and 16-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 16-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 16-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 16-1 Physical Properties

1. Name	2,3 Butylene Glycol (2,3 Butanediol)	1,3 Butylene Glycol (1,3 Butanediol)	1,4 Butylene Glycol (1,4 Butanediol)
2. Formula	C4H10O2	C4H10O2	C4H10O2
3. Molecular Weight, g/mol	90.122	90.122	90.122
4. Critical Temperature, K	611.00	643.00	667.00
5. Critical Pressure, bar	51.300	50.000	48.800
6. Critical Volume, ml/mol	267.00	292.00	297.00
7. Critical Compressibility Factor	0.270	0.273	0.261
8. Acentric Factor	1.1055	1.1456	1.1892
9. Melting Point, K	280.75	196.15	293.05
10. Boiling Point @ 1 atm, K	453.85	480.15	501.15
11. Heat of Vaporization @ BP, kJ/kg	612.35	627.86	692.71
12. Density of Liquid @ 25 C, g/ml	0.994	1.002	1.013
13. Surface Tension @ 25 C, dynes/cm	34.06	37.73	37.49
14. Heat Capacity of Gas @ 25 C, J/g K	1.43	1.41	1.37
15. Heat Capacity of Liquid @ 25 C, J/g K	2.36	2.26	2.24
16. Viscosity of Gas @ 25 C, micropoise	72.63	68.85	61.54
17. Viscosity of Liquid @ 25 C, centipoise	77.928	98.638	71.341
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.014	0.011	0.010
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.166	0.182	0.210
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-482.87	-435.15	-427.23
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-340.15	-292.86	-278.95
22. Flash Point, K	358.15	382.04	407.15
23. Autoignition Temperture, K	675.15	667.04	630.00
24. Lower Explosion Limit in Air, vol %	1.9	1.9	1.9
25. Upper Explosion Limit in Air, vol %	13.7	12.6	13.2
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

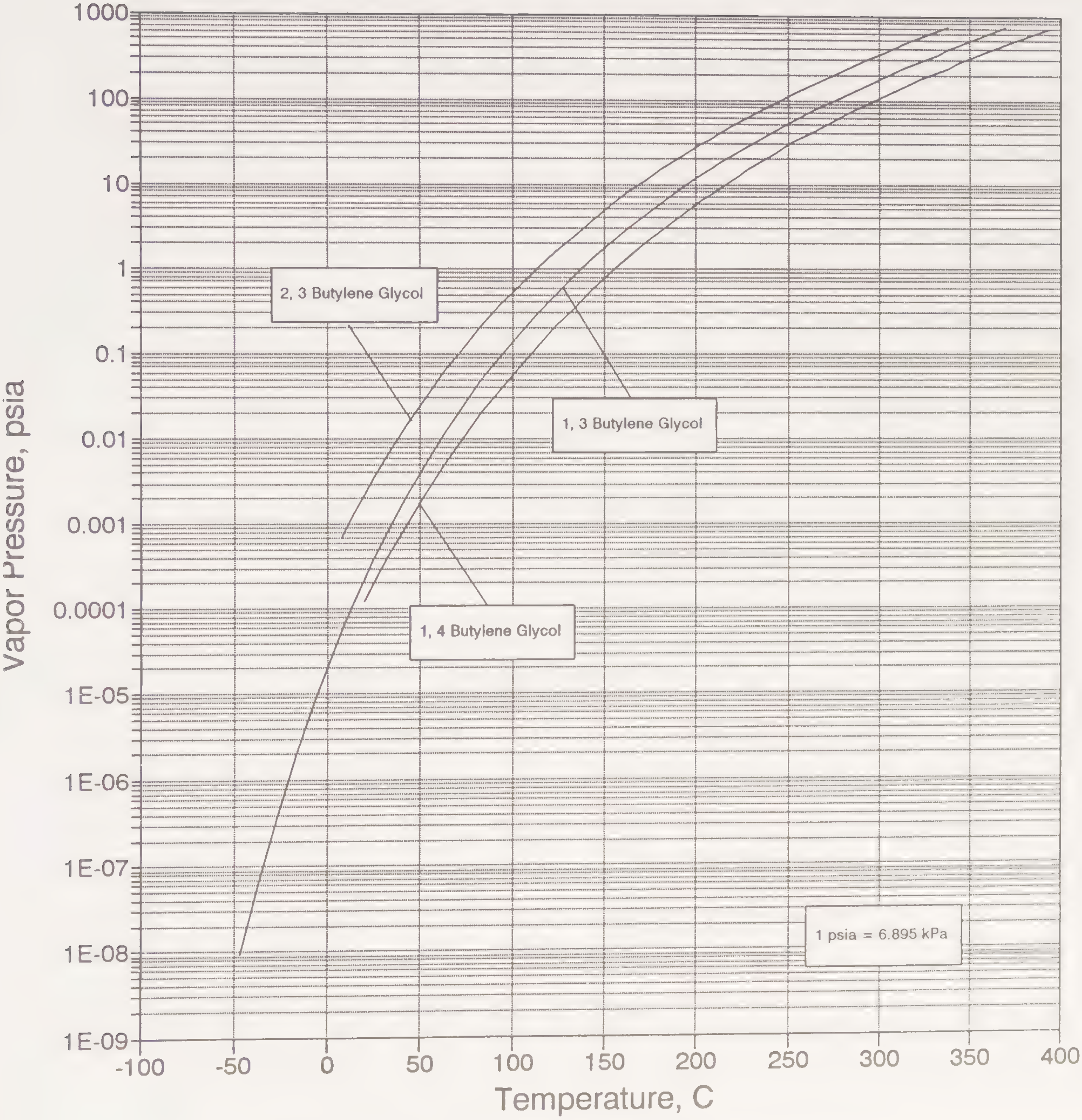

Figure 16-1 Vapor Pressure

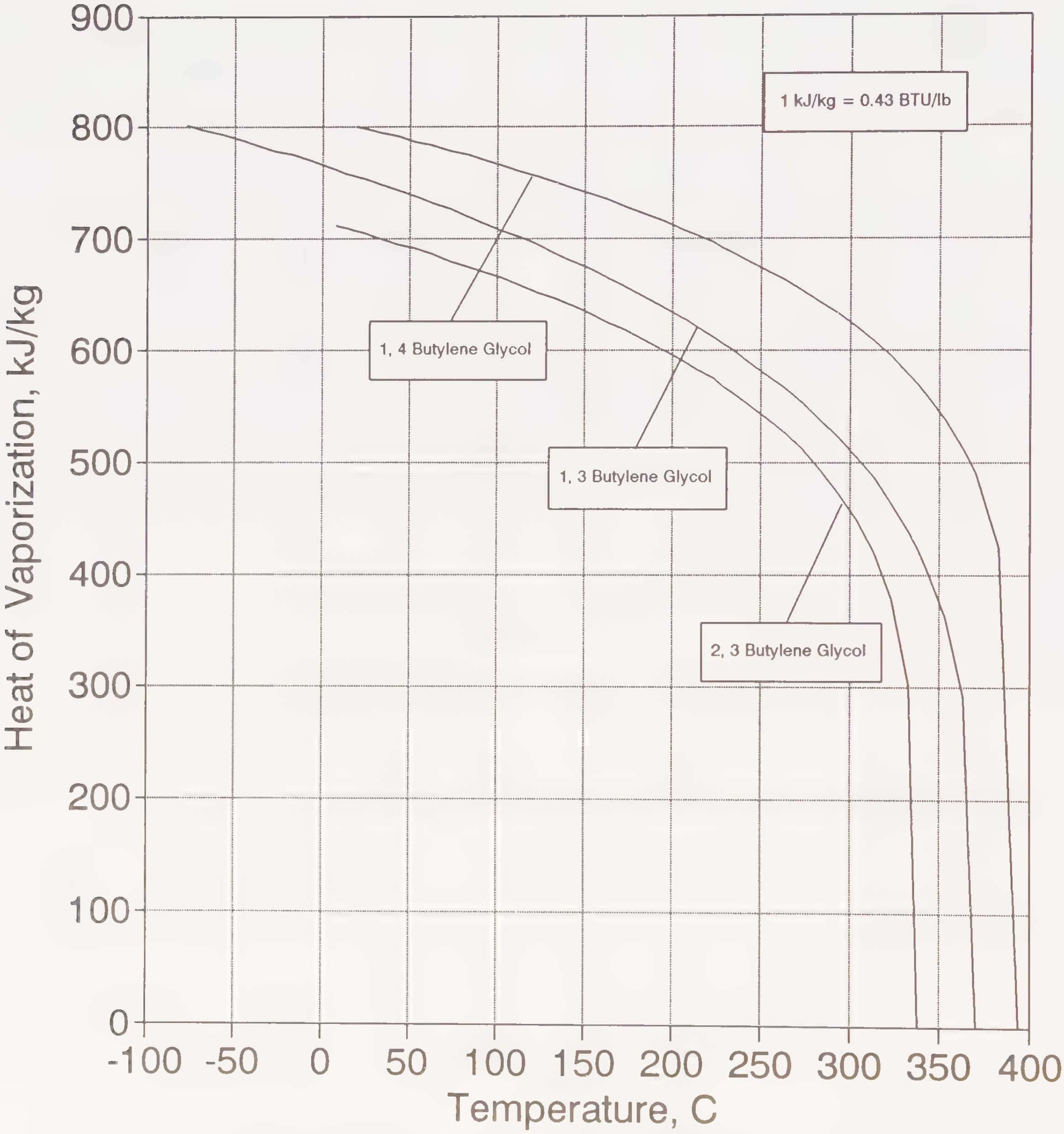

Figure 16-2 Heat of Vaporization

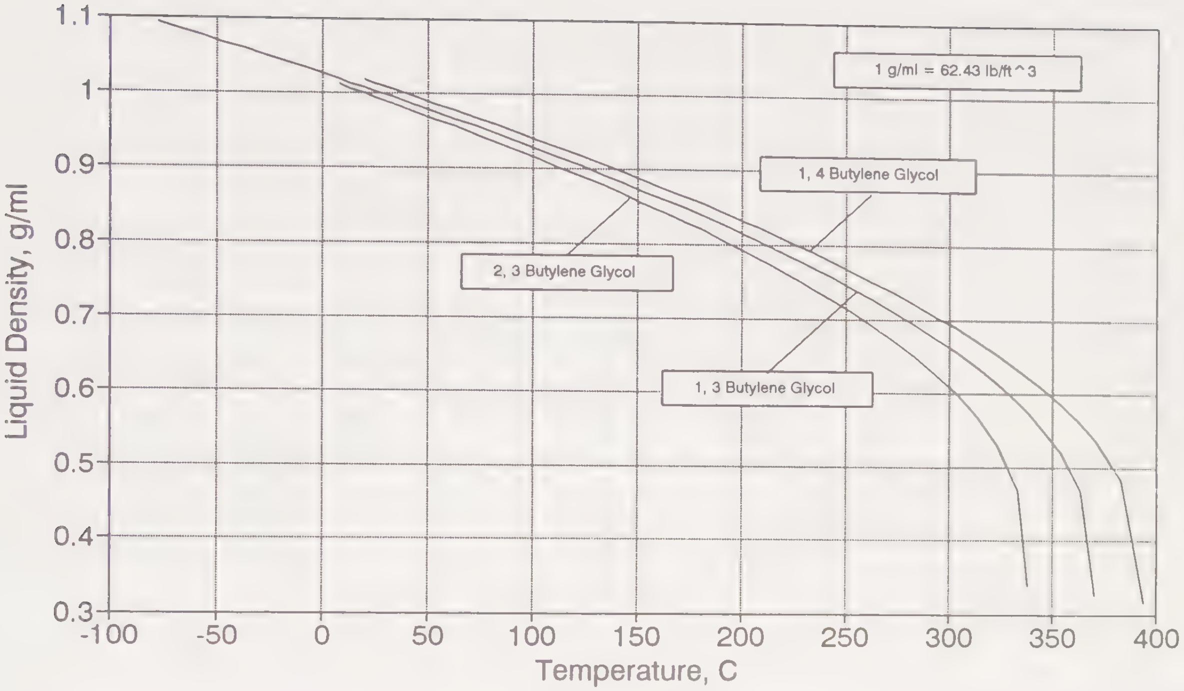

Figure 16-3 Liquid Density

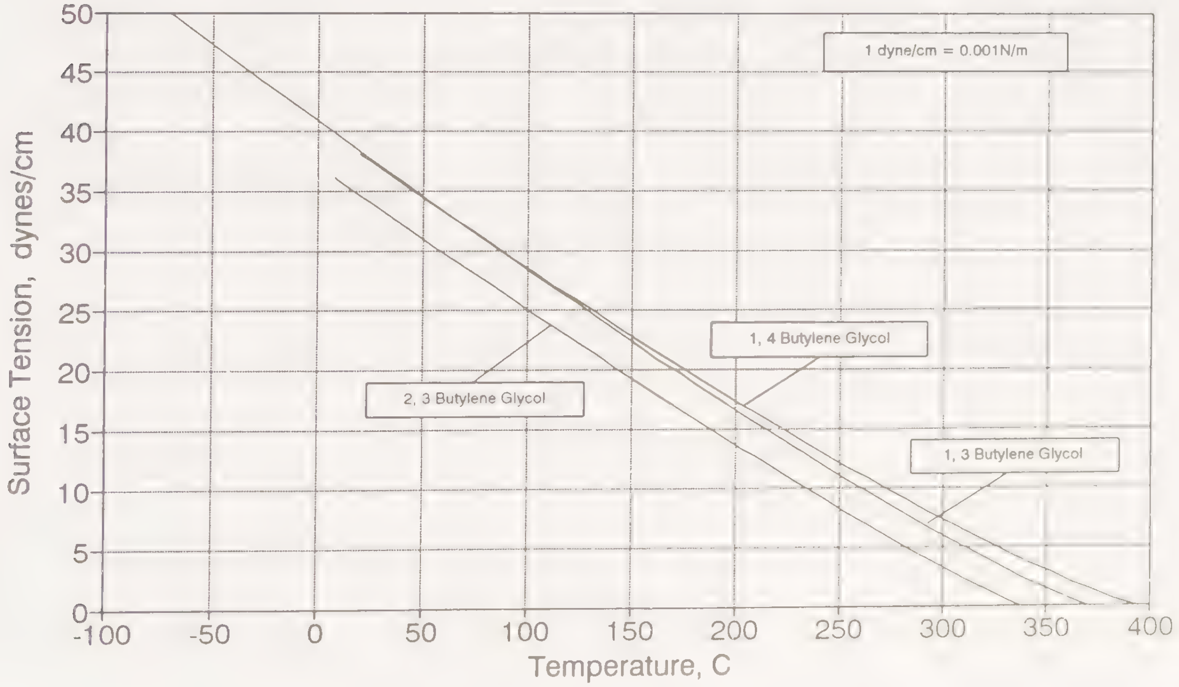

Figure 16-4 Surface Tension

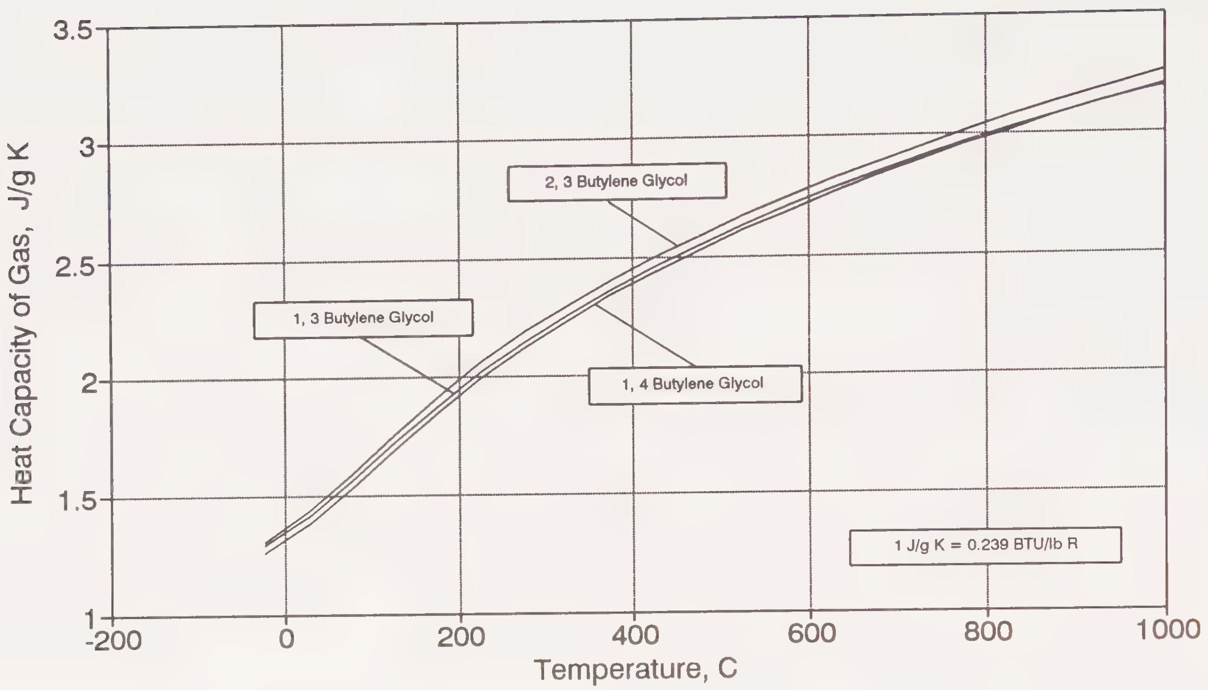

Figure 16-5 Heat Capacity of Gas

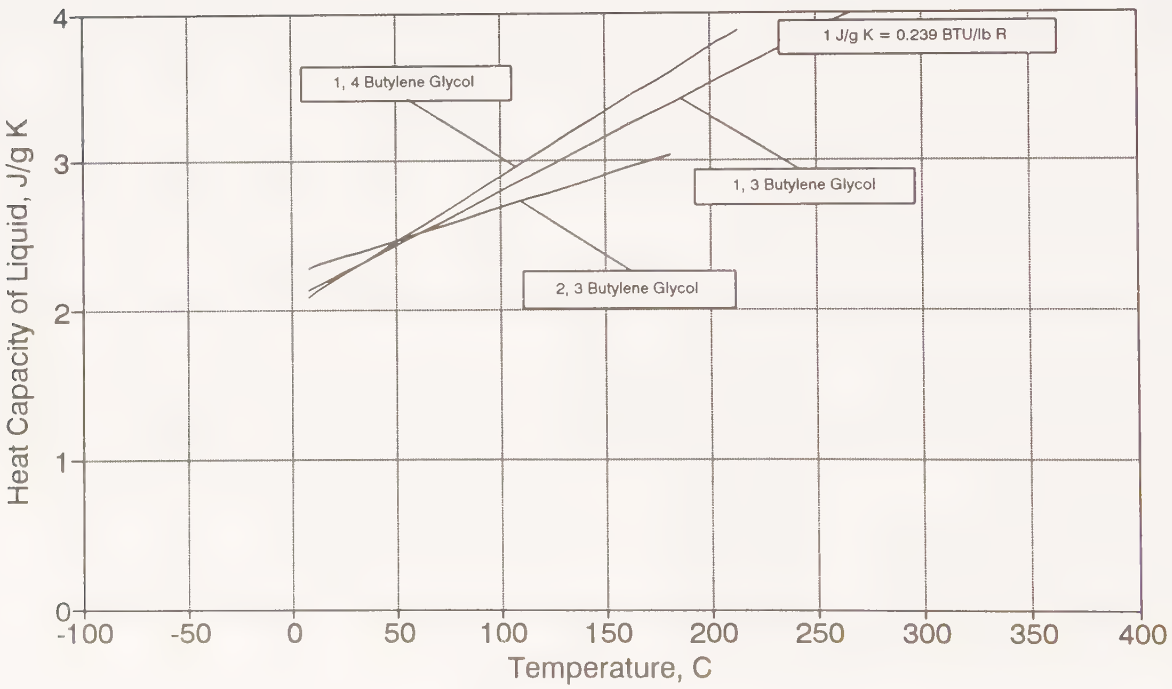

Figure 16-6 Heat Capacity of Liquid

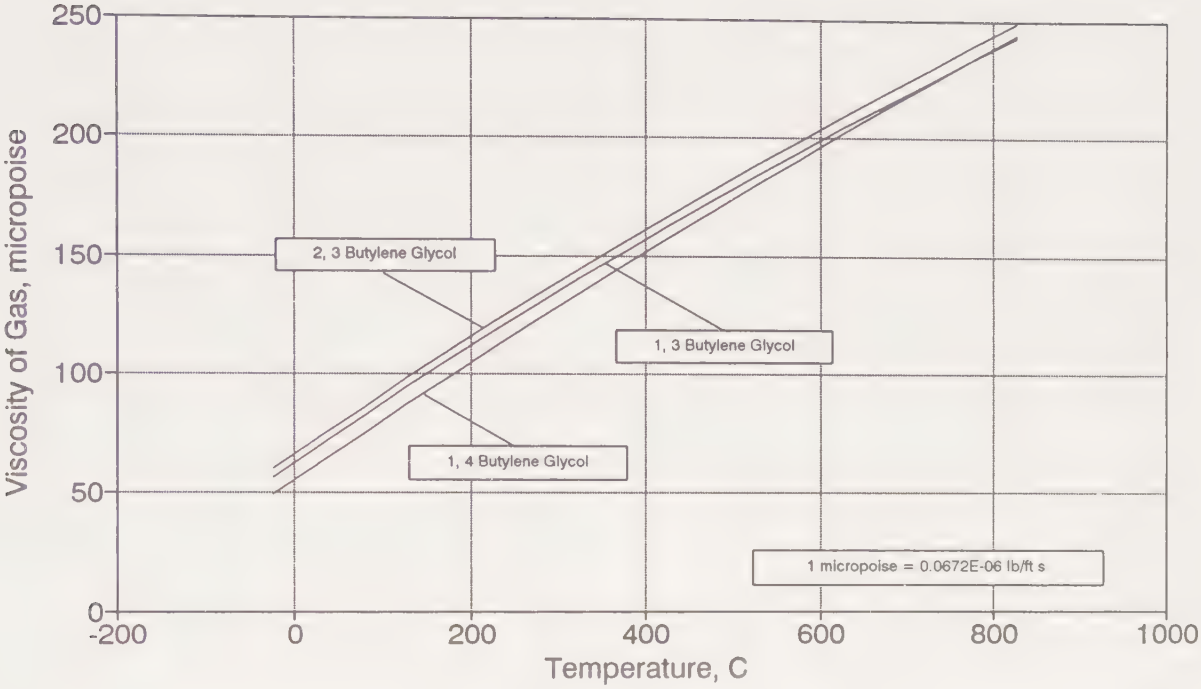

Figure 16-7 Viscosity of Gas

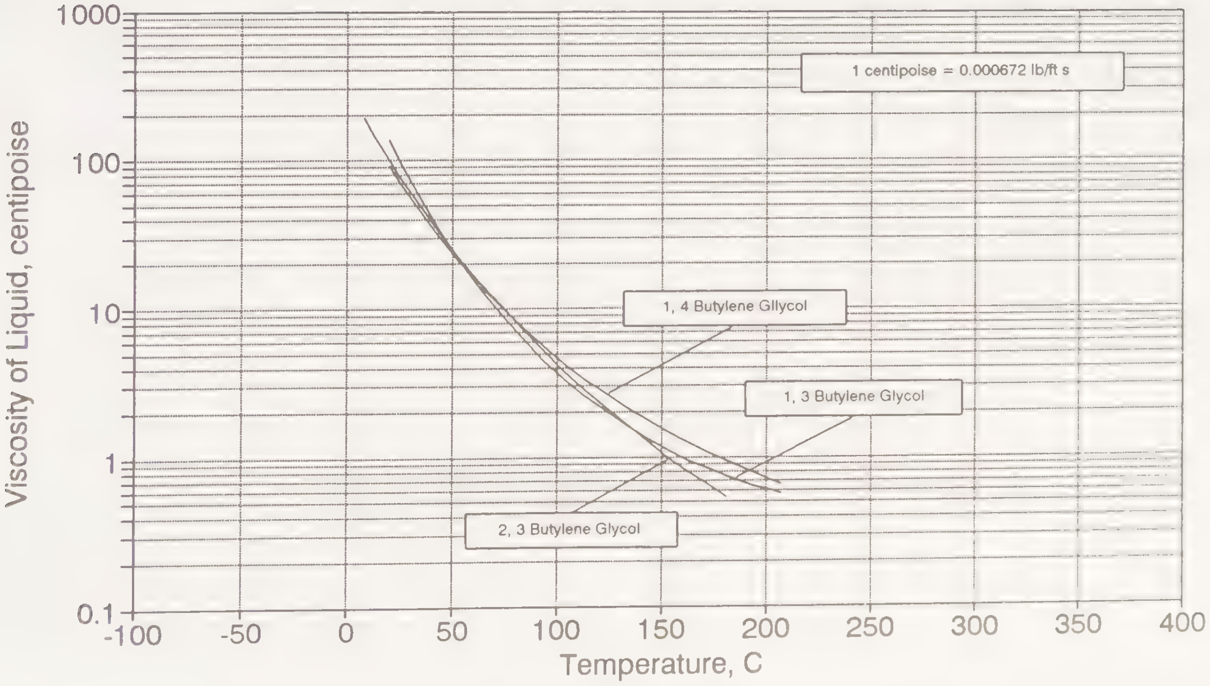

Figure 16-8 Viscosity of Liquid

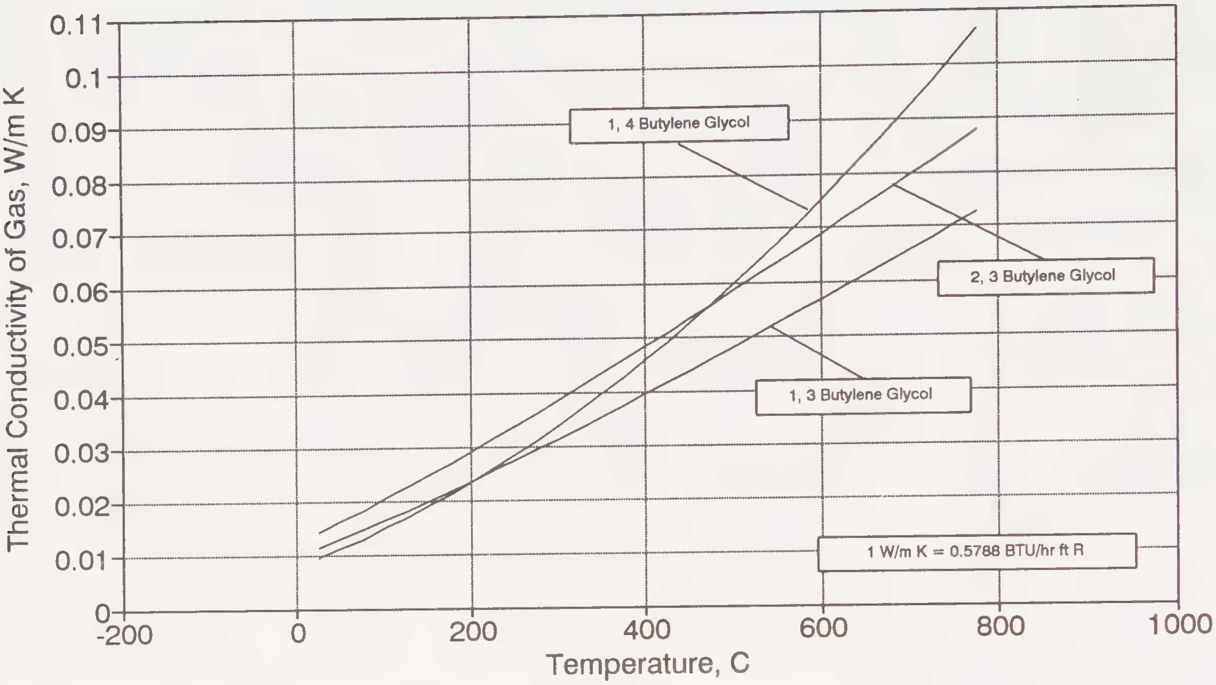

Figure 16-9 Thermal Conductivity of Gas

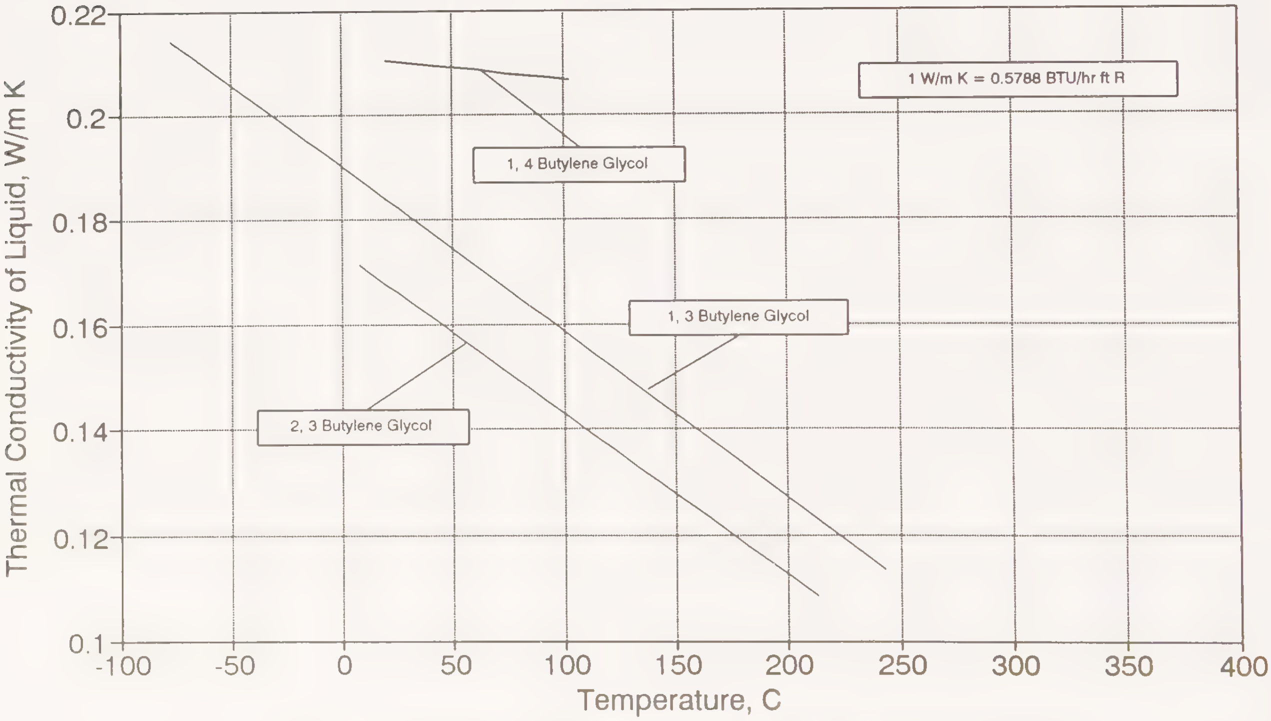

Figure 16-10 Thermal Conductivity of Liquid

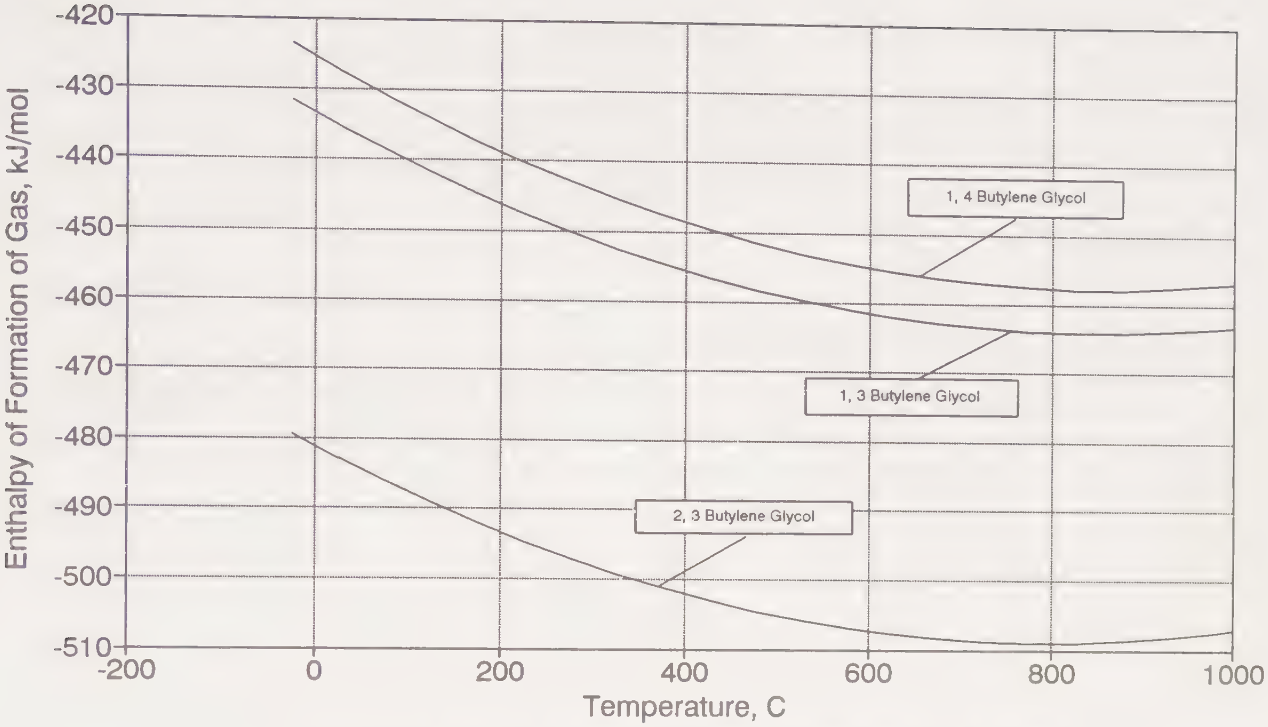

Figure 16-11 Enthalpy of Formation of Gas

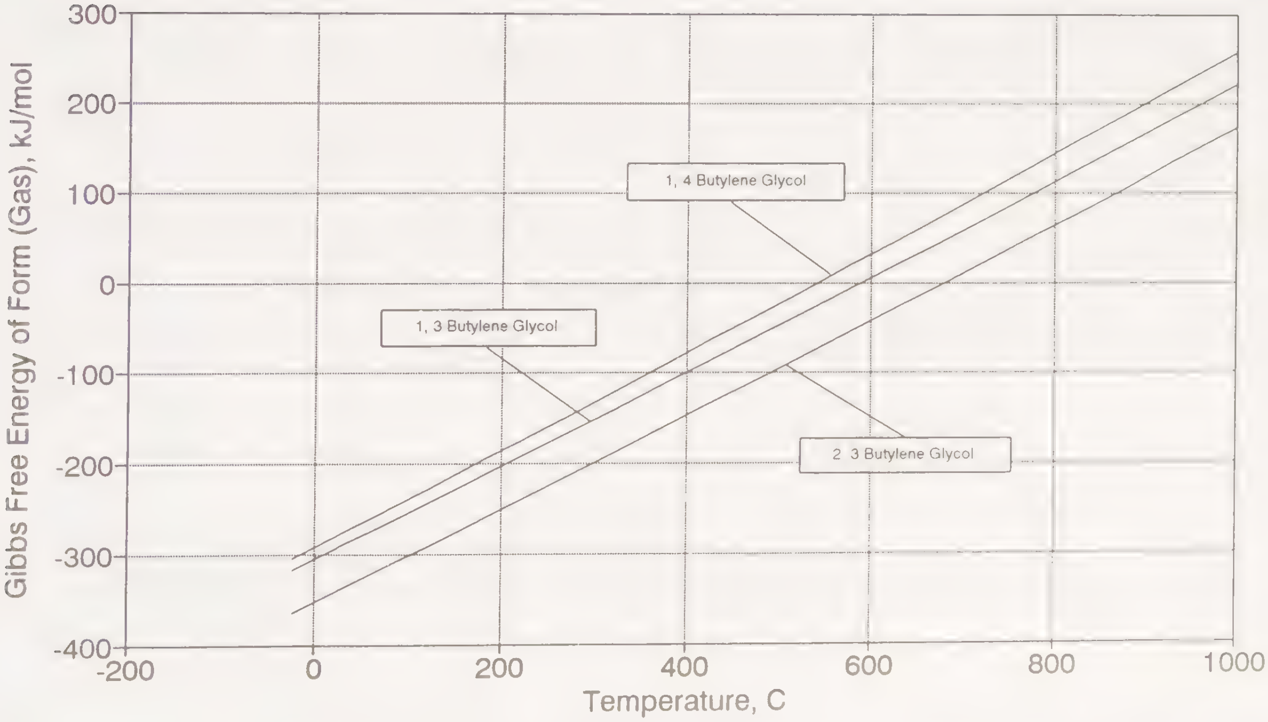

Figure 16-12 Gibbs Free Energy of Formation of Gas

Chapter 17

C_6 GLYCOLS

Robert W. Gallant and Carl L. Yaws

PHYSICAL PROPERTIES - Table 17-1

Property data from the literature (2,3,5,25,65,66,73,75,79,82,90,93,97,99,101) are given in Table 17-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 17-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 17-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is fair with possible errors of 10%.

LIQUID DENSITY - Figure 17-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 5% in most cases.

SURFACE TENSION - Figure 17-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 17-5 and 17-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was

accomplished using Equation (1-5a). Results are rough with errors of 25% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are rough with errors of 25% or less in most cases.

VISCOSITY - Figures 17-7 and 17-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 10% or less in most cases. A value of 616,000 centipoise at 223.15 K is given for hexylene glycol (5). This value appears to be very high.

THERMAL CONDUCTIVITY - Figures 17-9 and 17-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 17-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 17-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 17-1 Physical Properties

1. Name	Hexylene Glycol (2 Methyl 2,4 Pentanediol)	Hexamethylene Glycol (1,6 Hexanediol)
2. Formula	C6H14O2	C6H14O2
3. Molecular Weight, g/mol	118.176	118.176
4. Critical Temperature, K	621.0	670.0
5. Critical Pressure, bar	40.1	36.1
6. Critical Volume, ml/mol	398.0	398.0
7. Critical Compressibility Factor	0.309	0.258
8. Acentric Factor	1.1969	1.2675
9. Melting Point, K	223.15	315.15
10. Boiling Point @ 1 atm, K	470.65	516.15
11. Heat of Vaporization @ BP, kJ/kg	519.47	560.41
12. Density of Liquid @ 25 C, g/ml	0.918	0.755 @ BP
13. Surface Tension @ 25 C, dynes/cm	15.77	13.35 @ BP
14. Heat Capacity of Gas @ 25 C, J/g K	1.468	1.430
15. Heat Capacity of Liquid @ 25 C, J/g K	2.84	3.33 @ BP
16. Viscosity of Gas @ 25 C, micropoise	64.09	61.57
17. Viscosity of Liquid @ 25 C, centipoise	------	0.019 @ BP
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.0115	0.0099
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.1522	0.1136 @ BP
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-535.75	-470.57
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-328.57	-268.17
22. Flash Point, K	366.0	372.04
23. Autoignition Temperature, K	579.0	------
24. Lower Explosion Limit in Air, vol %	1.3	1.3
25. Upper Explosion Limit in Air, vol %	9.0	9.2
26. Solubility in Water @ 25 C, ppm(wt)	------	------

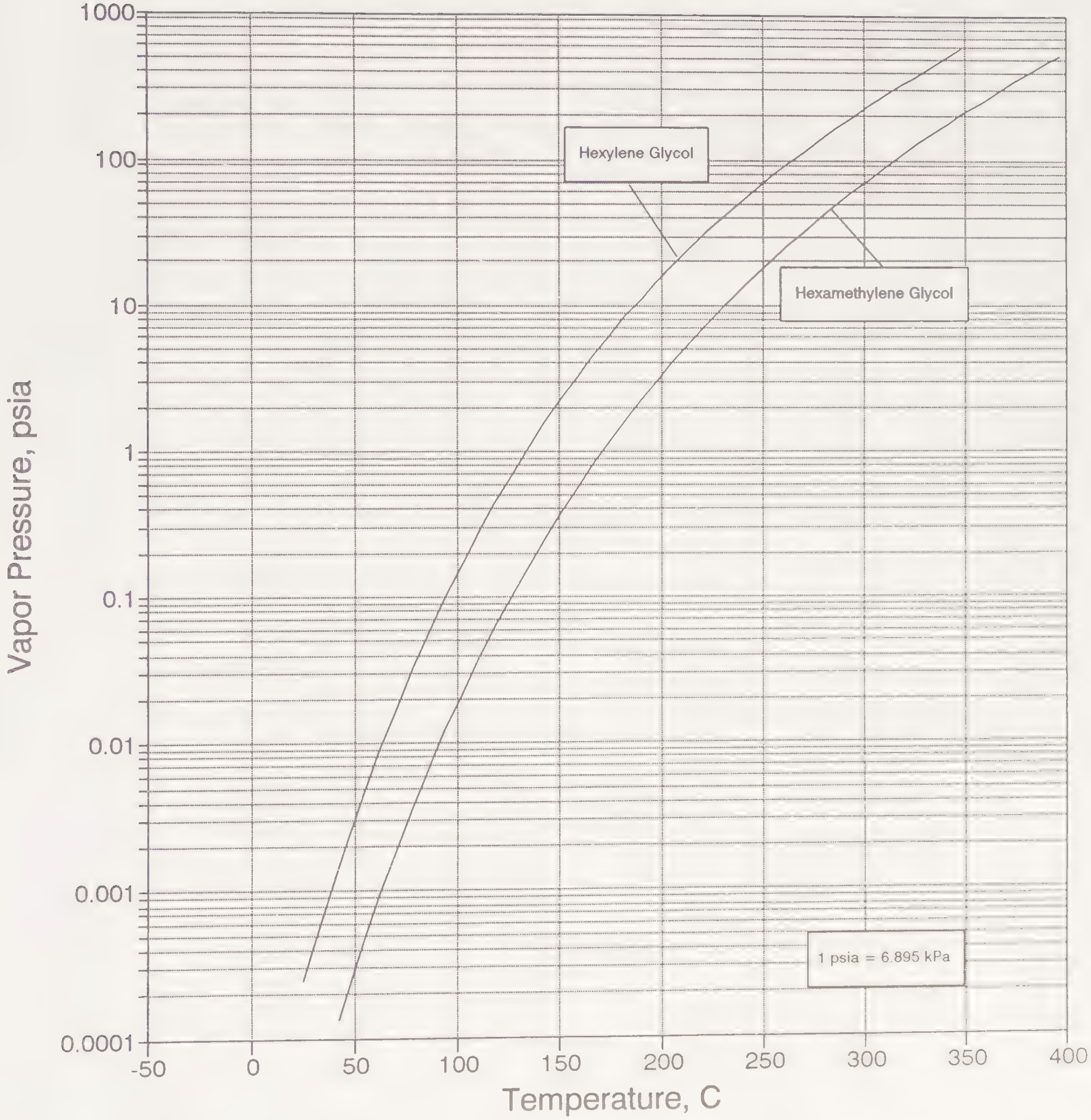

Figure 17-1 Vapor Pressure

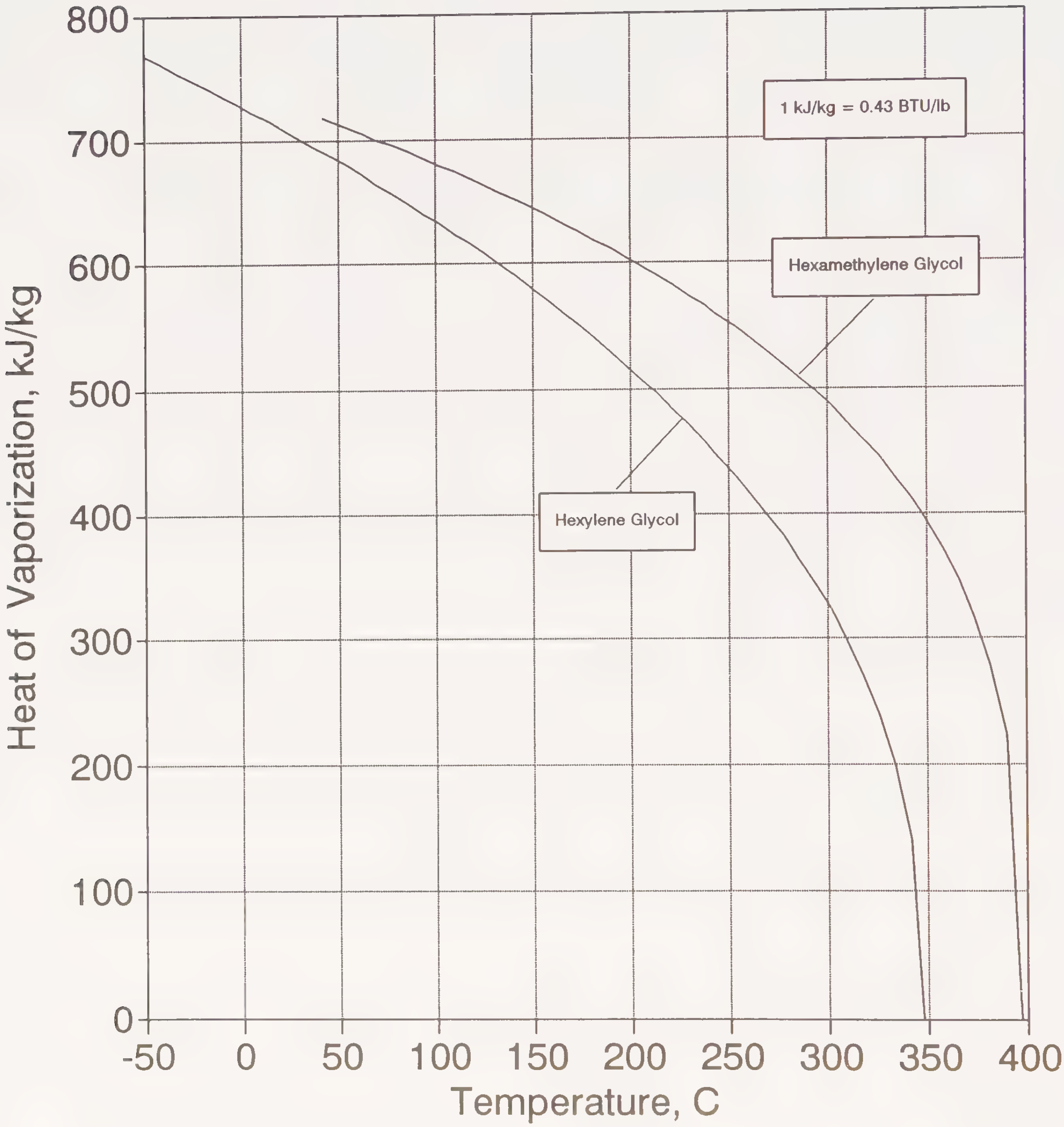

Figure 17-2 Heat of Vaporization

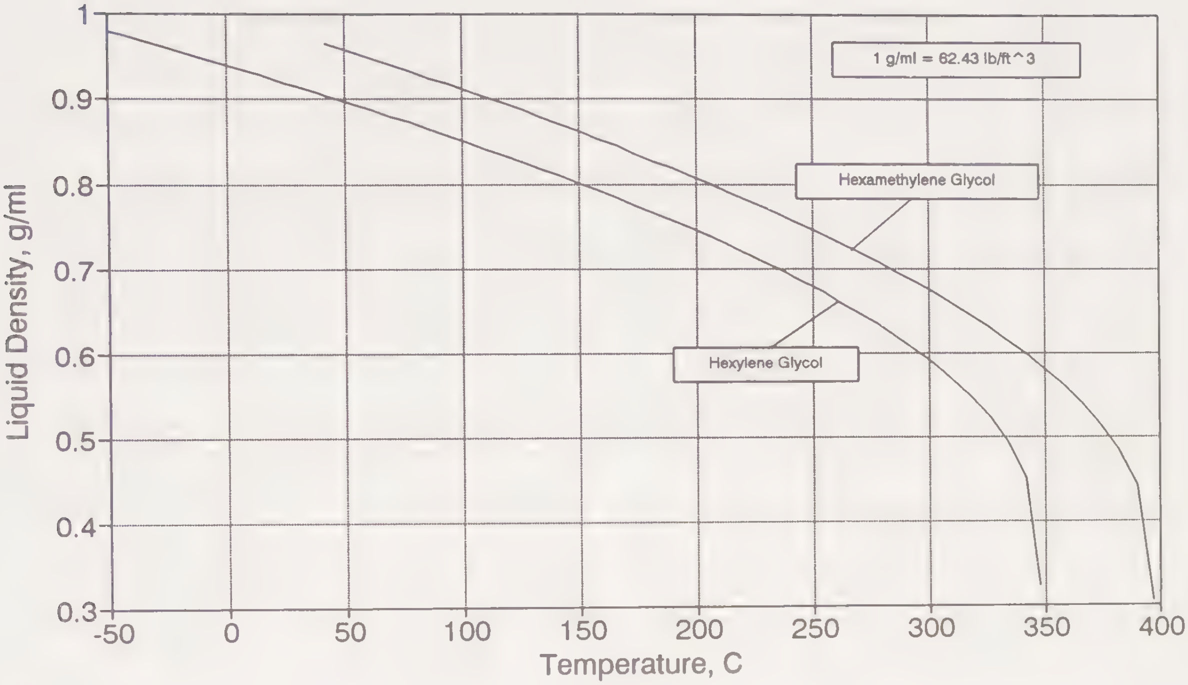

Figure 17-3 Liquid Density

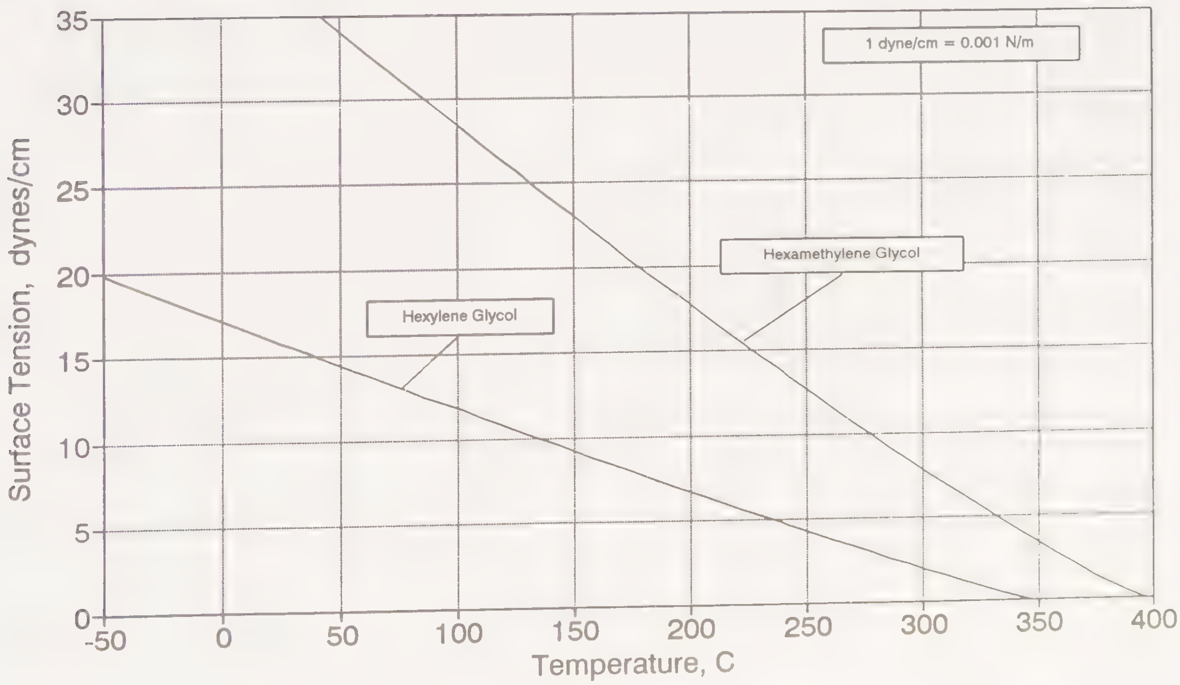

Figure 17-4 Surface Tension

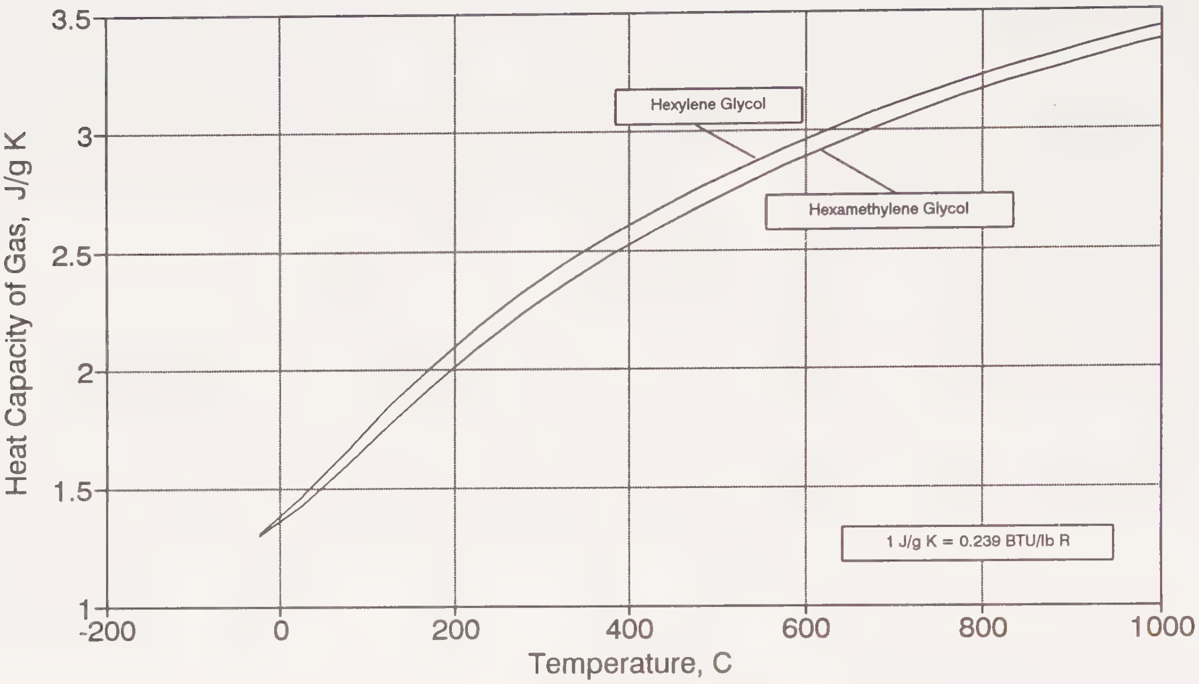

Figure 17-5 Heat Capacity of Gas

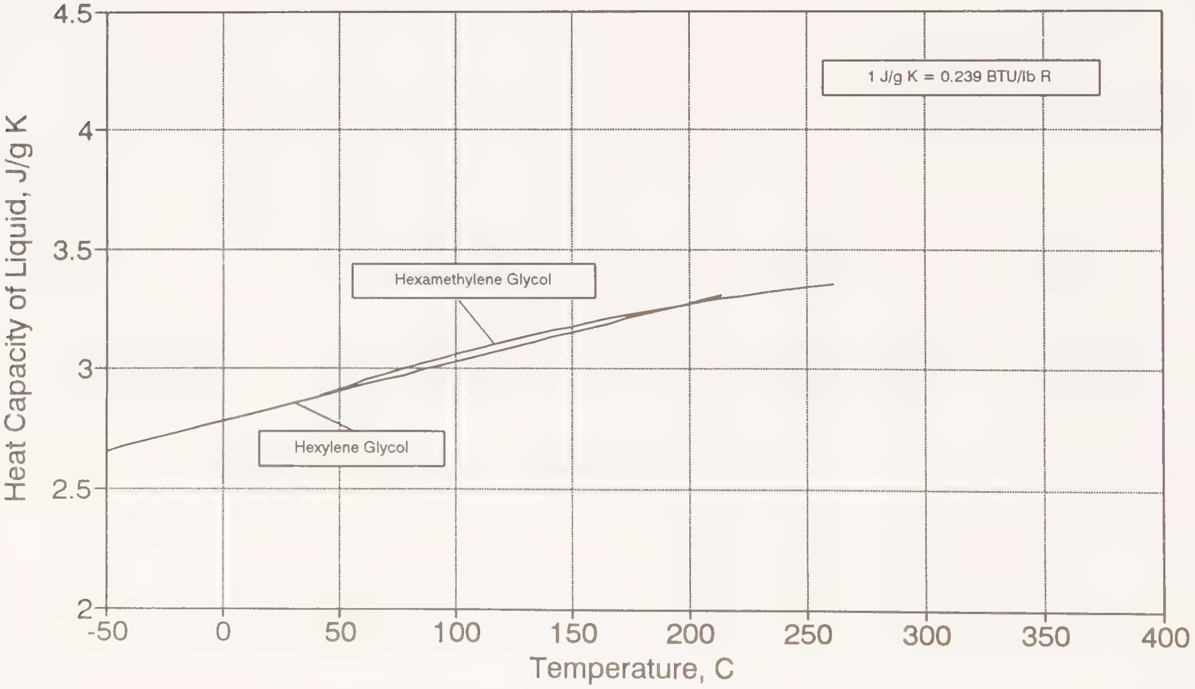

Figure 17-6 Heat Capacity of Liquid

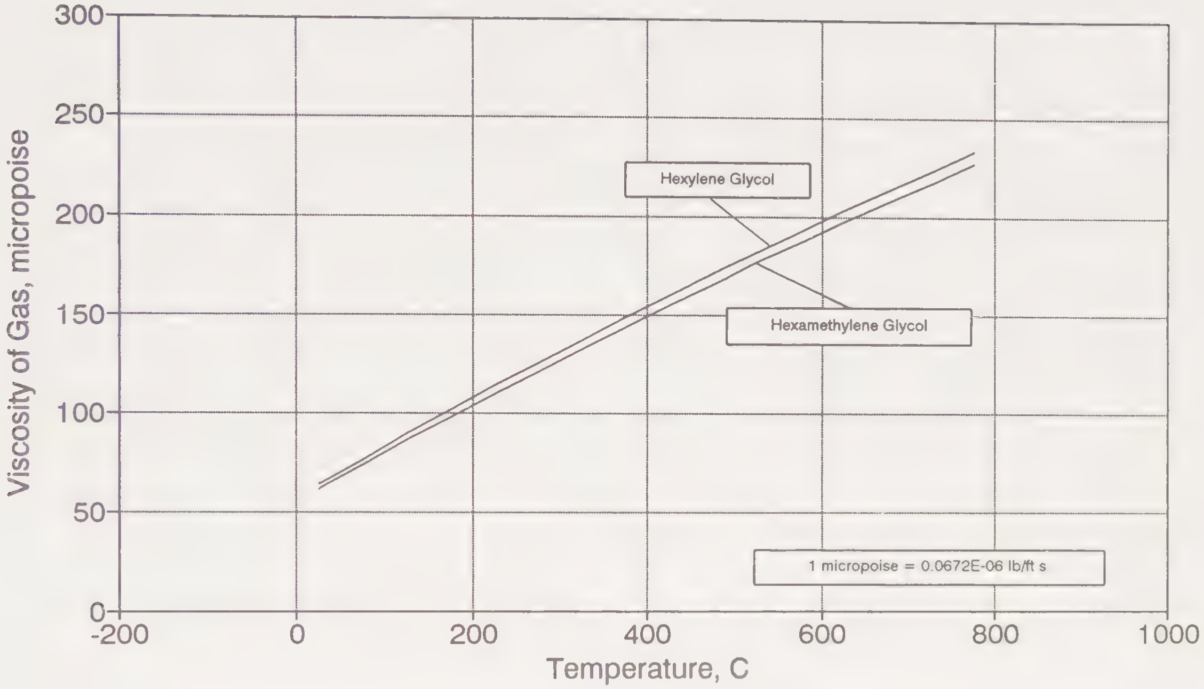

Figure 17-7 Viscosity of Gas

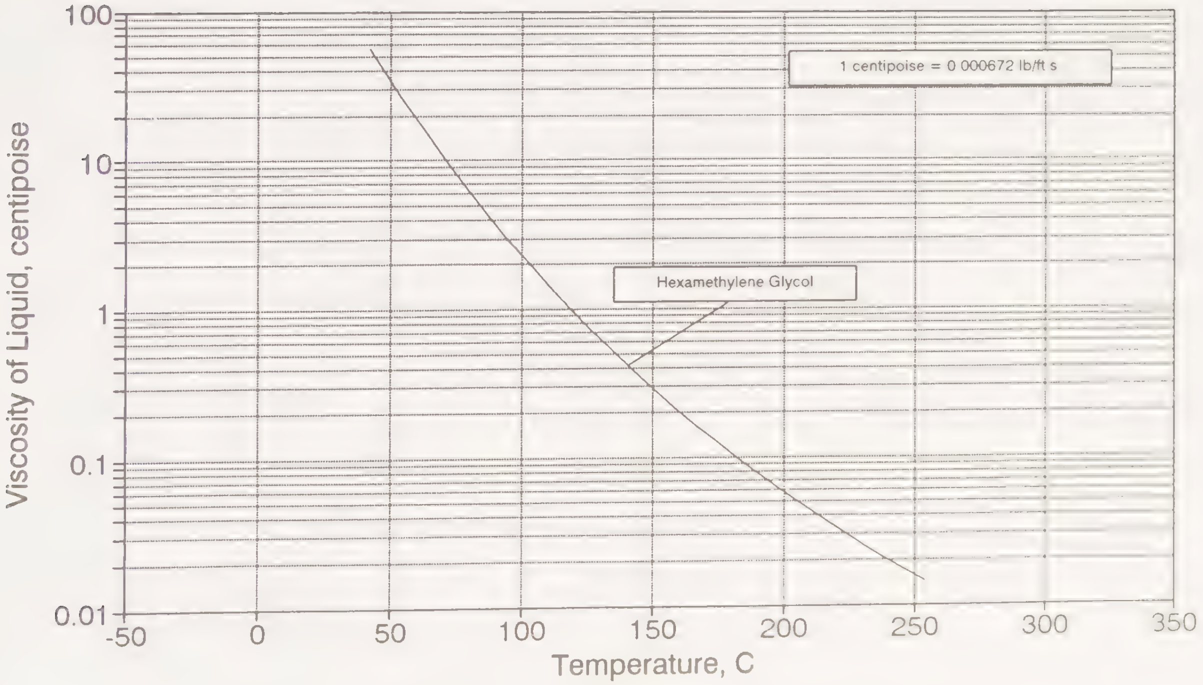

Figure 17-8 Viscosity of Liquid

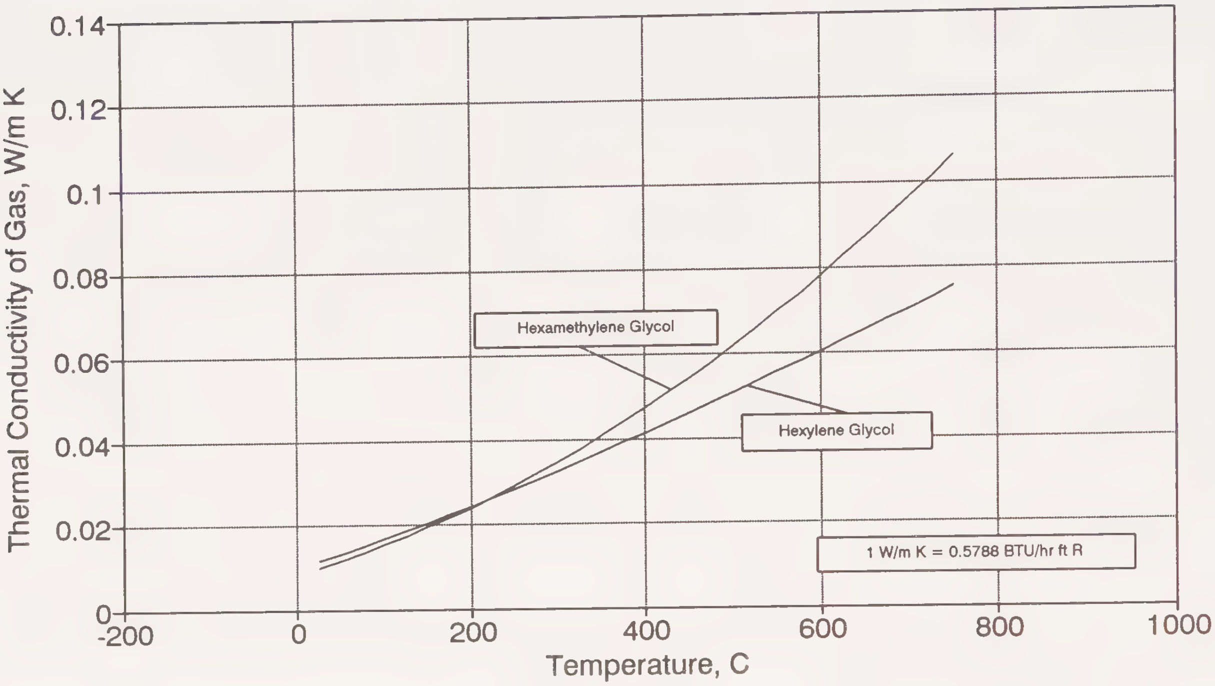

Figure 17-9 Thermal Conductivity of Gas

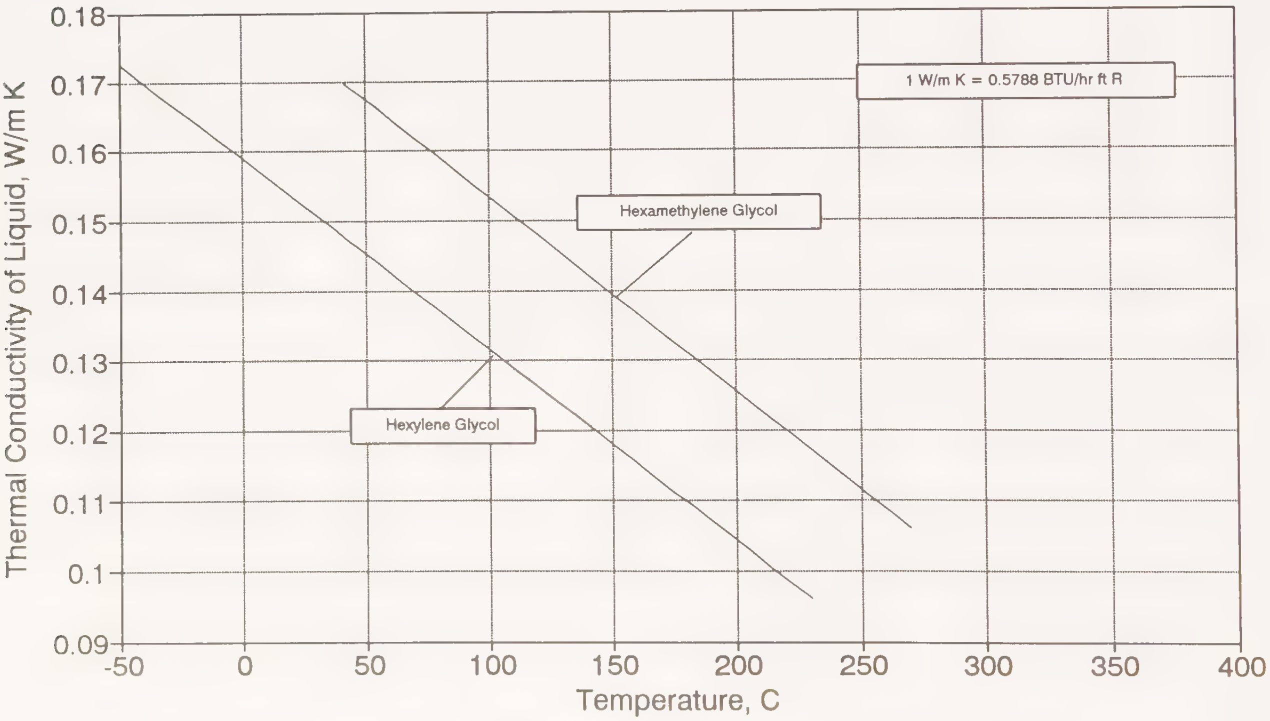

Figure 17-10 Thermal Conductivity of Liquid

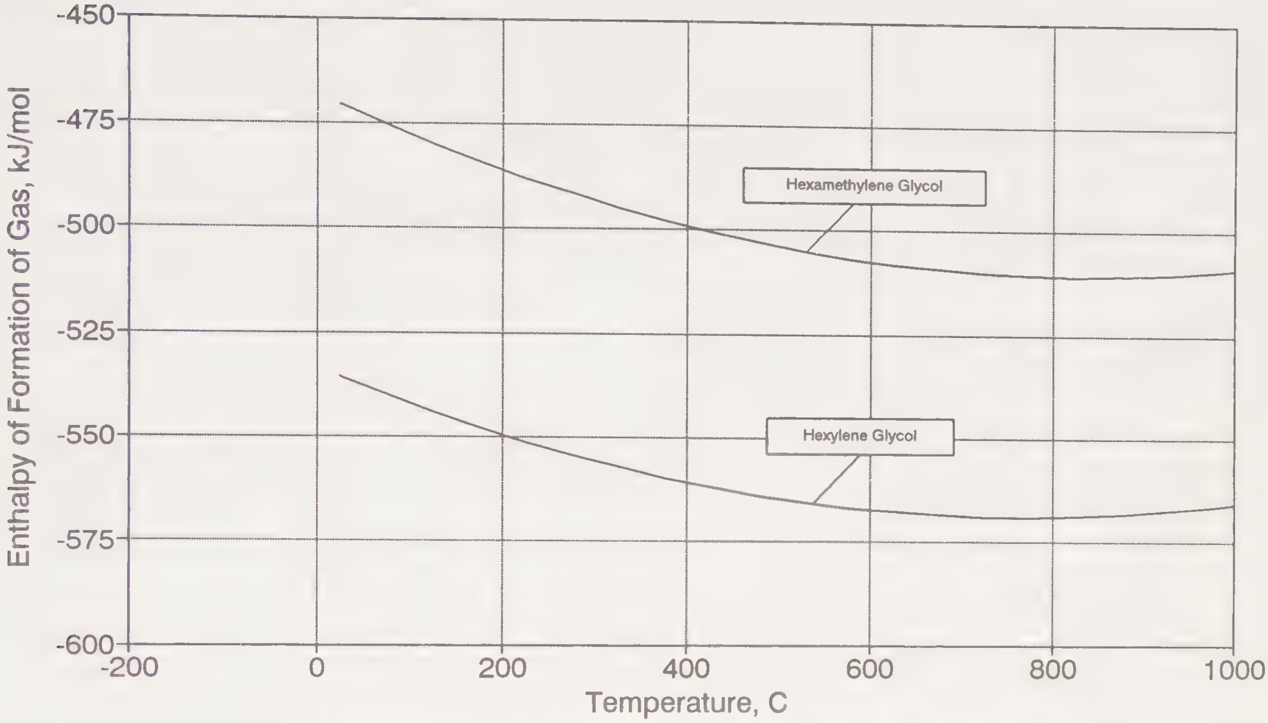

Figure 17-11 Enthalpy of Formation of Gas

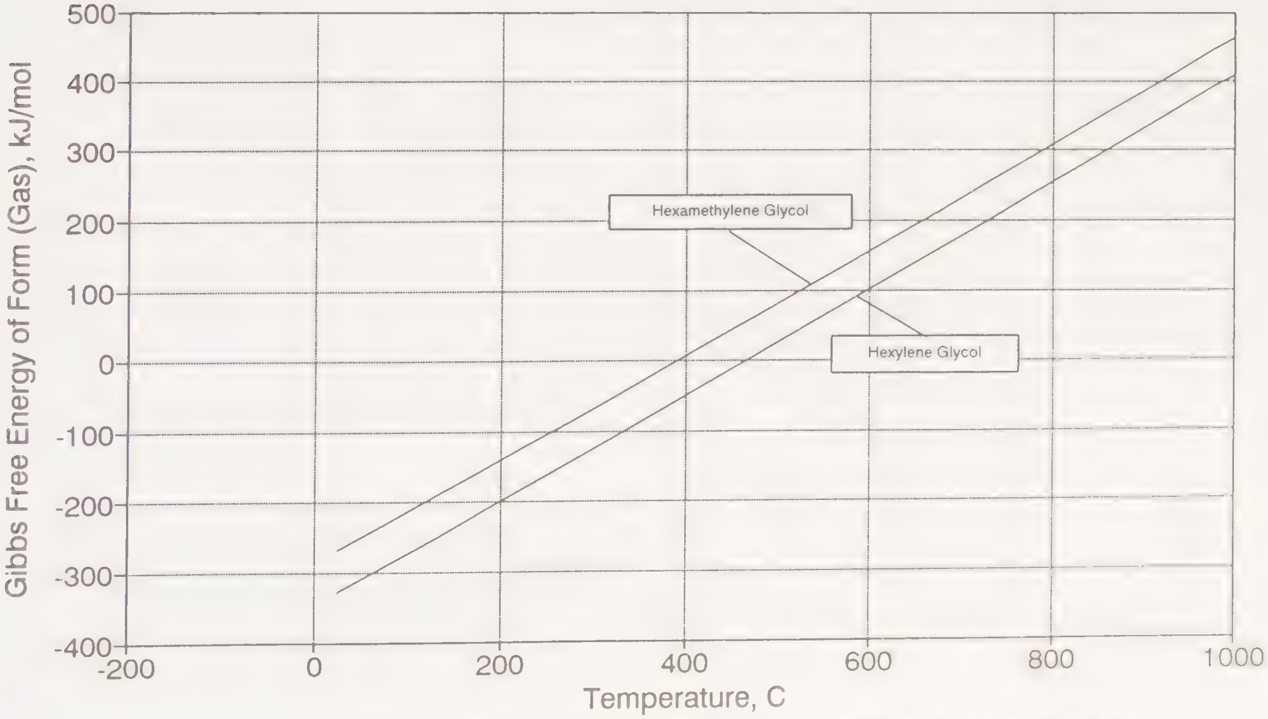

Figure 17-12 Gibbs Free Energy of Formation of Gas

Chapter 18

PROPYLAMINES

Robert W. Gallant, Carl L. Yaws and Li Bu

PHYSICAL PROPERTIES - Table 18-1

Property data from the literature (2,3,8,21,23,26,36,38,63-65,68,75,77,82,103,120,132,157,167-175) are given in Table 18-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation, lower explosion limit in air and solubility in water are also available.

VAPOR PRESSURE - Figure 18-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 10% or less in most cases.

HEAT OF VAPORIZATION - Figure 18-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with errors of about 5%.

LIQUID DENSITY - Figure 18-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

SURFACE TENSION - Figure 18-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 18-5 and 18-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 10% or less in most cases.

VISCOSITY - Figures 18-7 and 18-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 5% or less in most cases.

THERMAL CONDUCTIVITY - Figures 18-9 and 18-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 10% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 18-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C (5,14) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 18-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C (5) were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 18-1 Physical Properties

1. Name	Propylamine	Dipropylamine	Tripropylamine
2. Formula	C3H9N	C6H15N	C9H21N
3. Molecular Weight, g/mol	59.111	101.192	143.272
4. Critical Temperature, K	496.95	555.80	577.50
5. Critical Pressure, bar	47.420	36.300	22.300
6. Critical Volume, ml/mol	260.00	418.00	576.00
7. Critical Compressibility Factor	0.298	0.328	0.268
8. Acentric Factor	0.2957	0.4646	0.6994
9. Melting Point, K	190.15	210.15	179.65
10. Boiling Point @ 1 atm, K	321.65	382.00	429.65
11. Heat of Vaporization @ BP, kJ/kg	499.68	347.28	252.66
12. Density of Liquid @ 25 C, g/ml	0.714	0.737	0.754
13. Surface Tension @ 25 c, dynes/cm	22.49	22.22	22.39
14. Heat Capacity of Gas @ 25 C, J/g K	1.61	1.56	1.58
15. Heat Capacity of Liquid @ 25 C, J/g K	2.78	2.14	2.01
16. Viscosity of Gas @ 25 C, micropoise	70.99	63.56	61.01
17. Viscosity of Liquid @ 25 C, centipoise	0.385	0.515	0.621
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.015	0.012	0.012
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.173	0.129	0.119
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-72.91	-117.00	-162.49
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	38.66	84.96	131.19
22. Flash Point, K	260.93	290.15	302.04
23. Autoignition Temperture, K	590.93	572.15	------
24. Lower Explosion Limit in Air, vol %	2.0	1.1	0.8
25. Upper Explosion Limit in Air, vol %	10.4	7.7	5.4
26. Solubility in Water @ 25 C, ppm(wt)	total	------	------

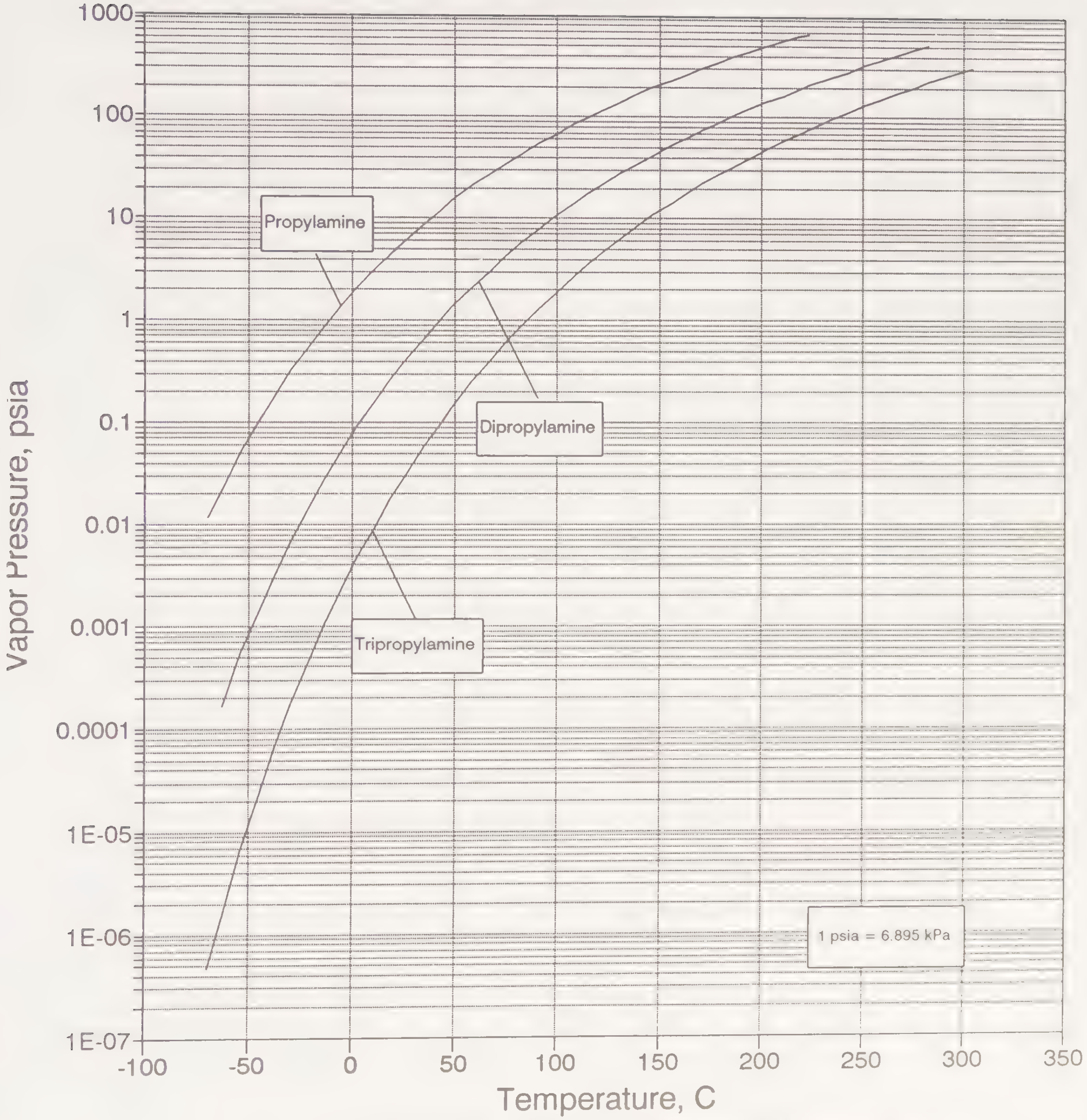

Figure 18-1 Vapor Pressure

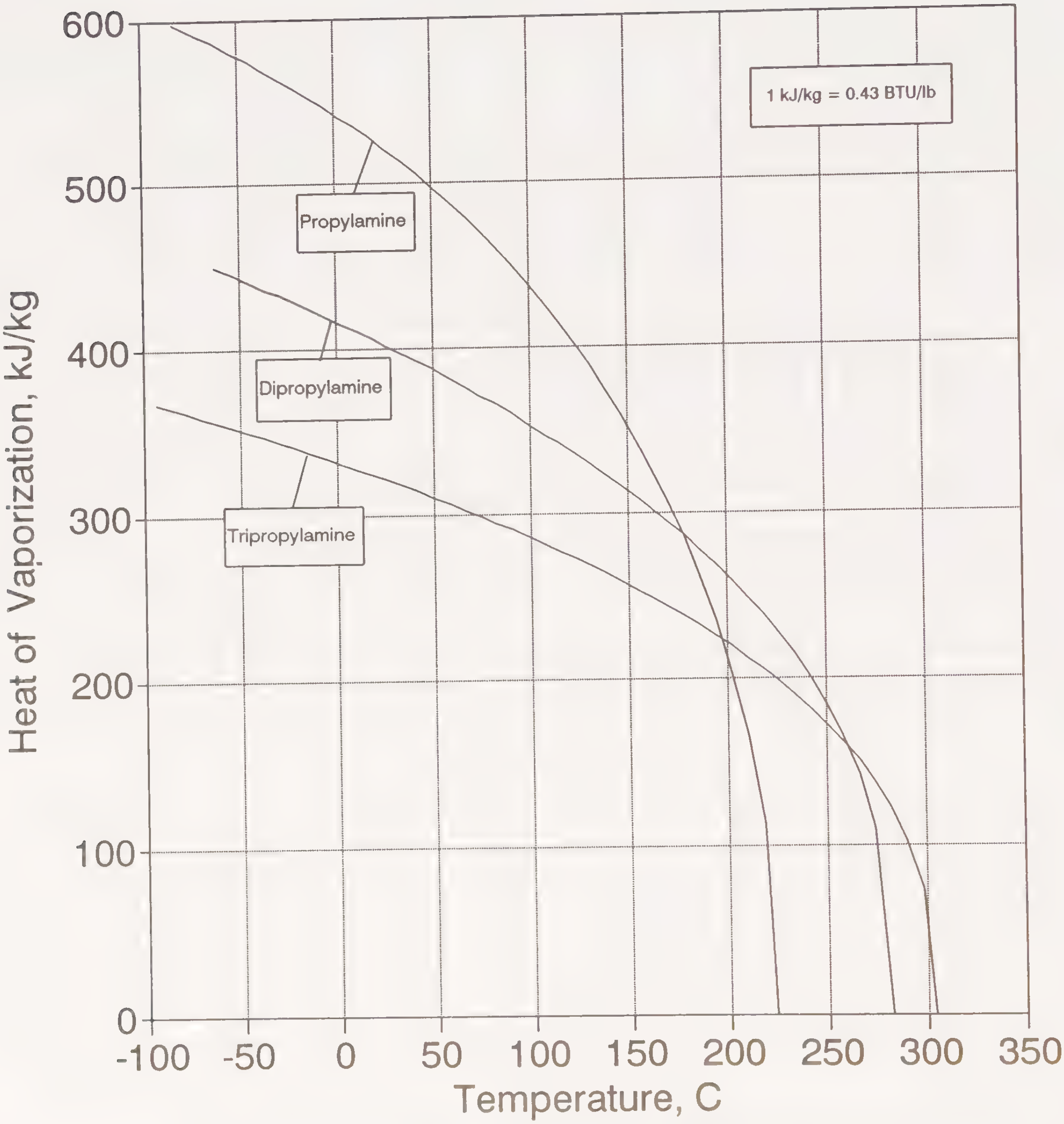

Figure 18-2 Heat of Vaporization

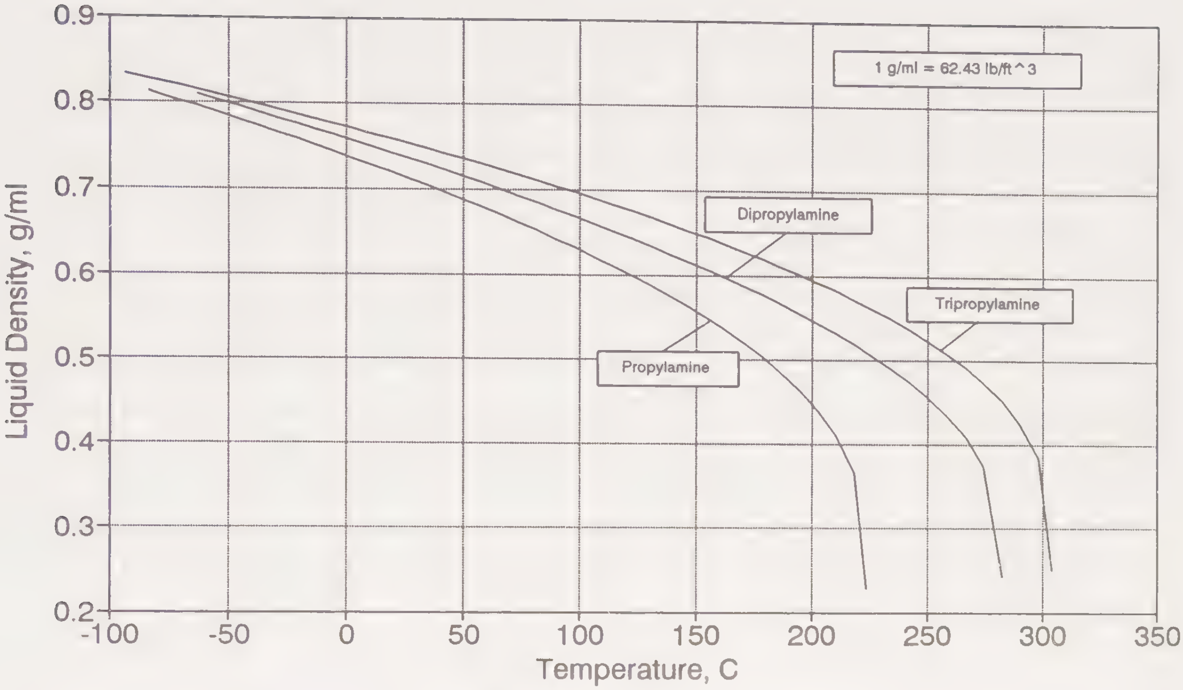

Figure 18-3 Liquid Density

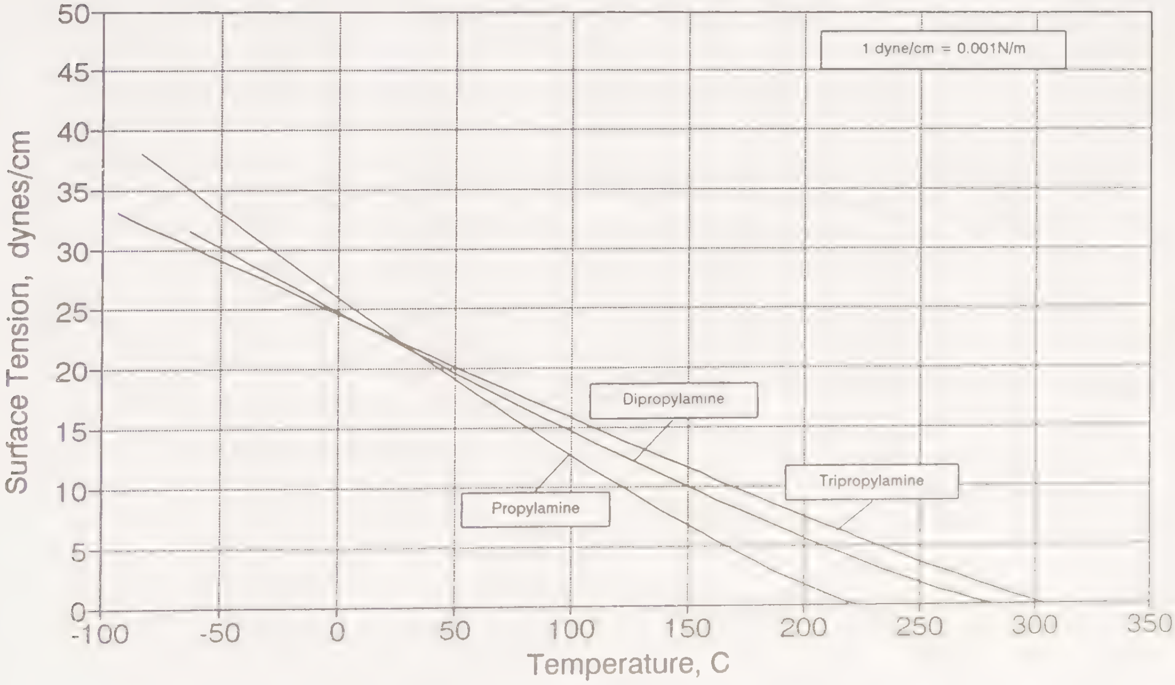

Figure 18-4 Surface Tension

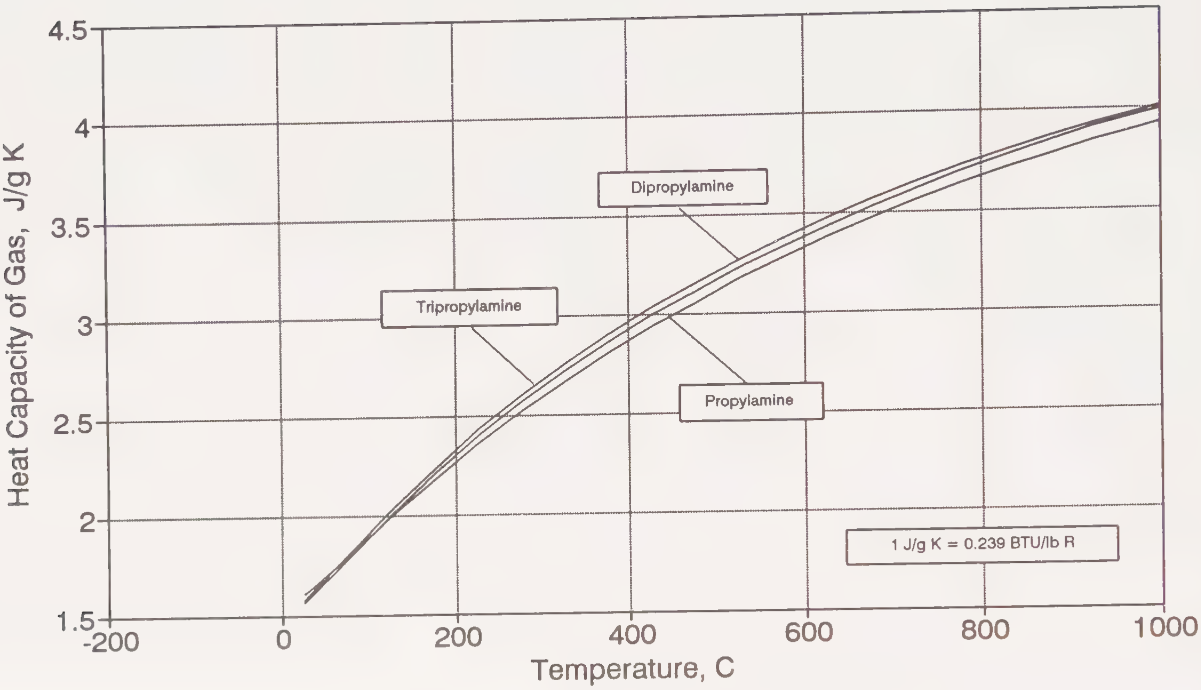

Figure 18-5 Heat Capacity of Gas

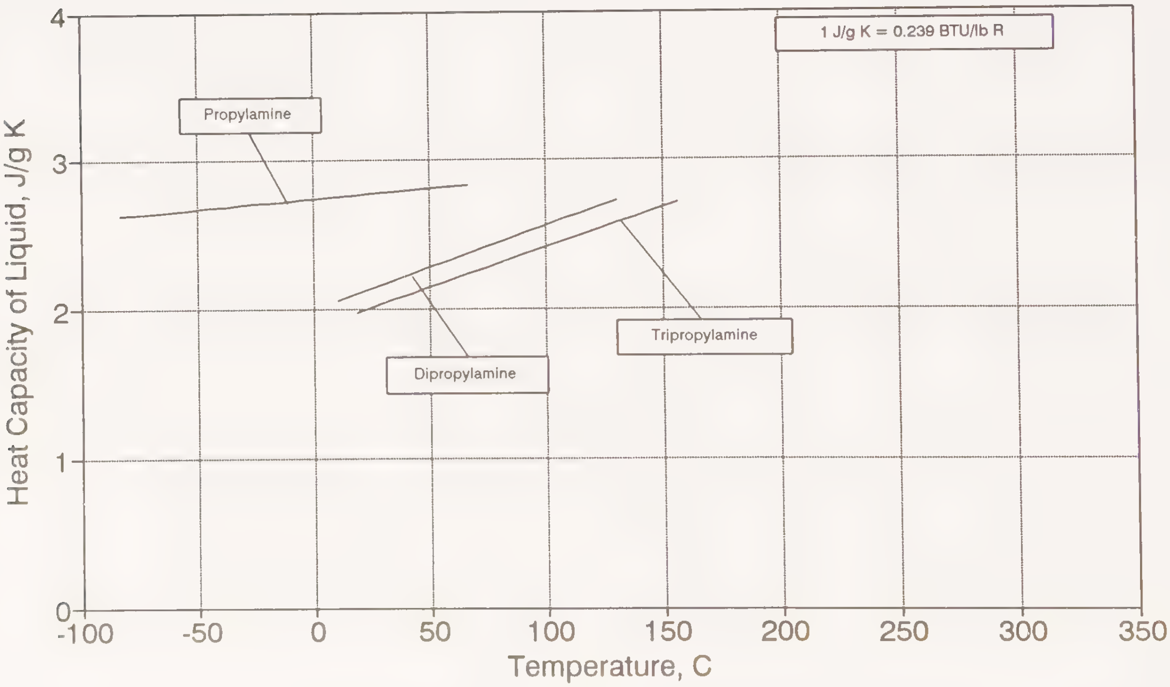

Figure 18-6 Heat Capacity of Liquid

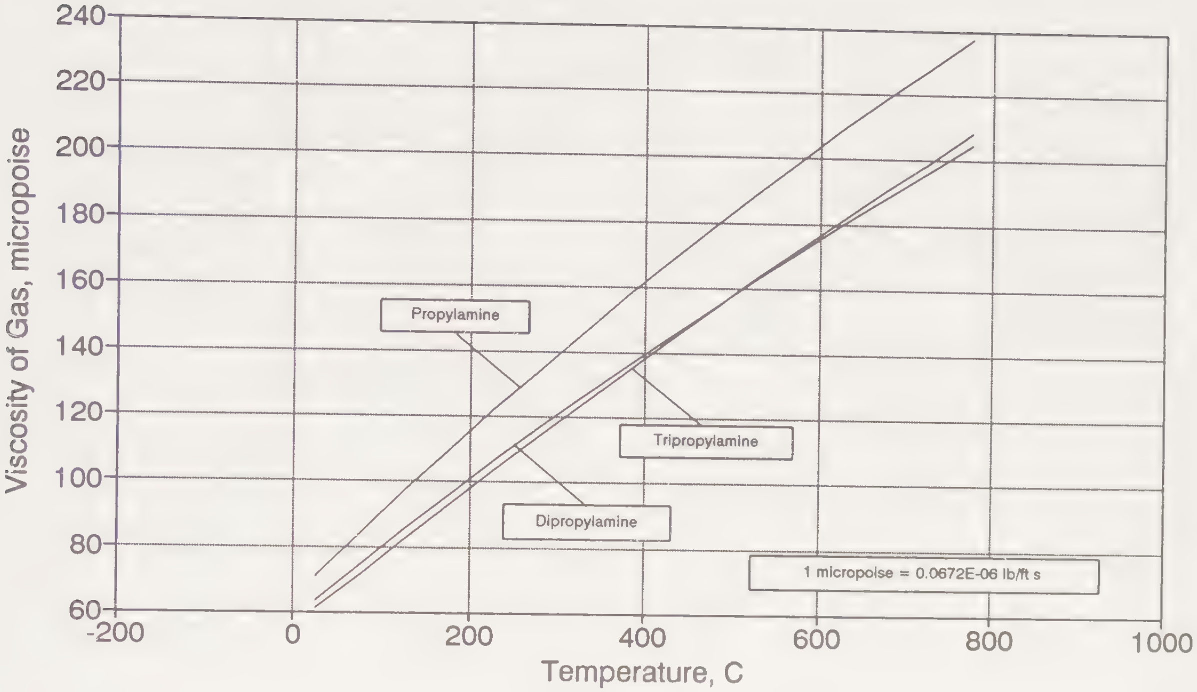

Figure 18-7 Viscosity of Gas

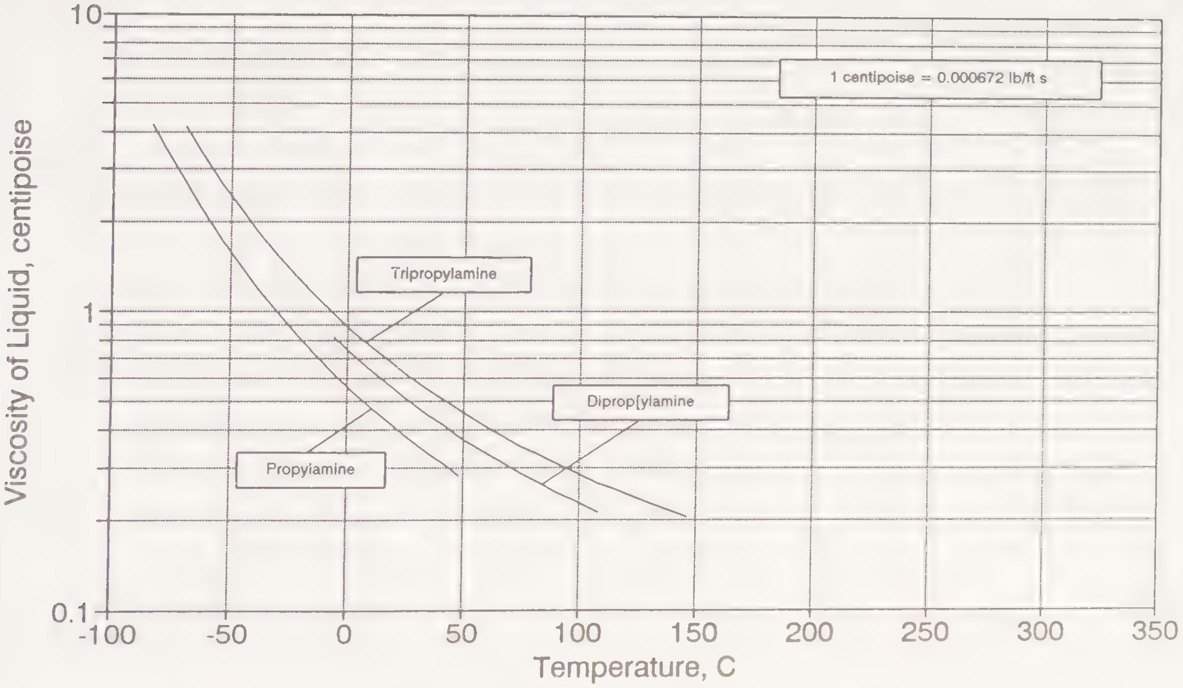

Figure 18-8 Viscosity of Liquid

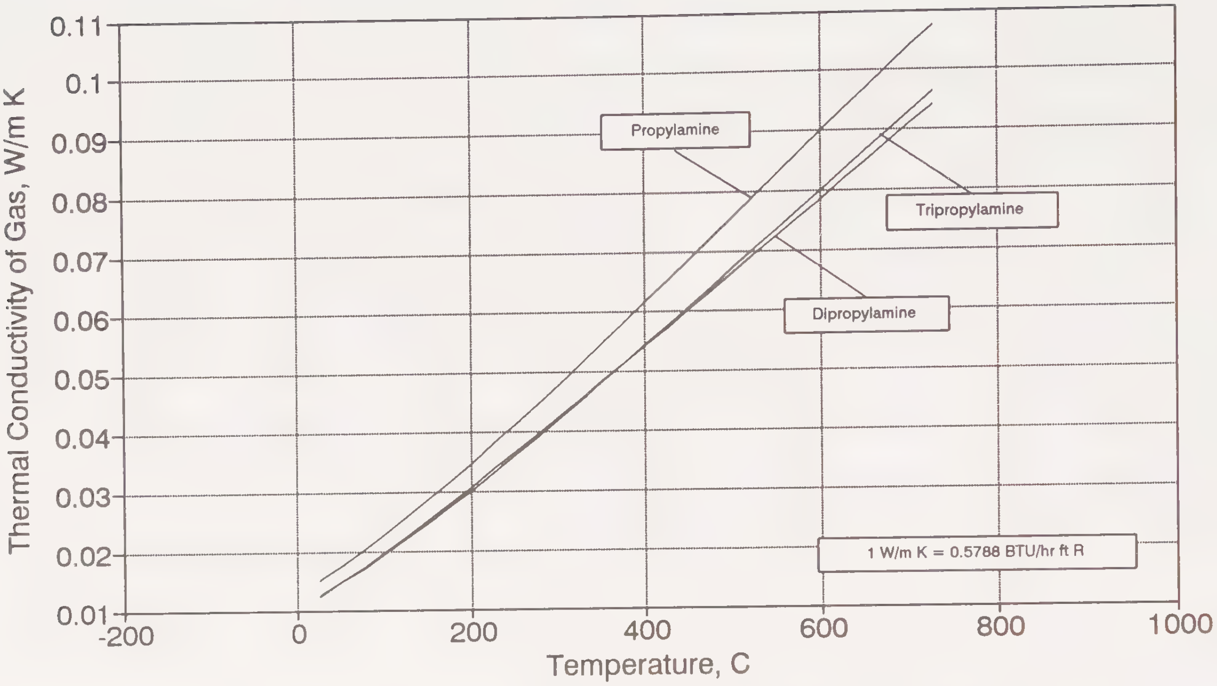

Figure 18-9 Thermal Conductivity of Gas

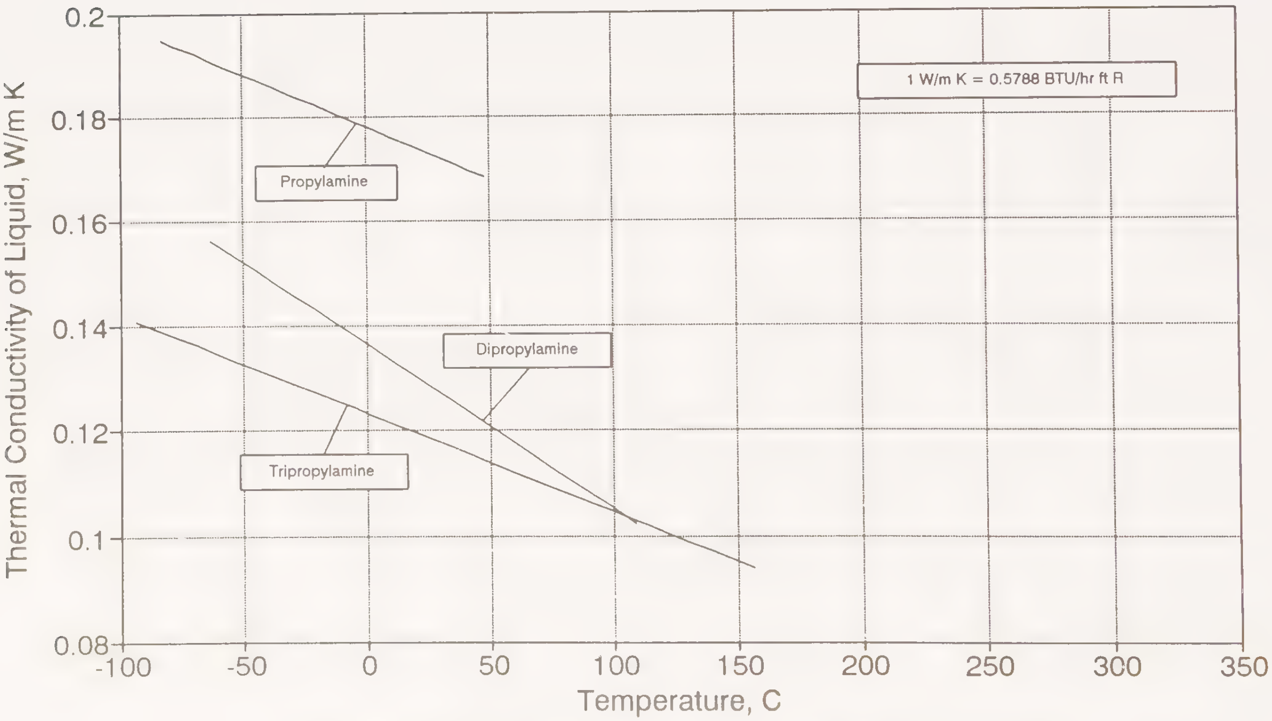

Figure 18-10 Thermal Conductivity of Liquid

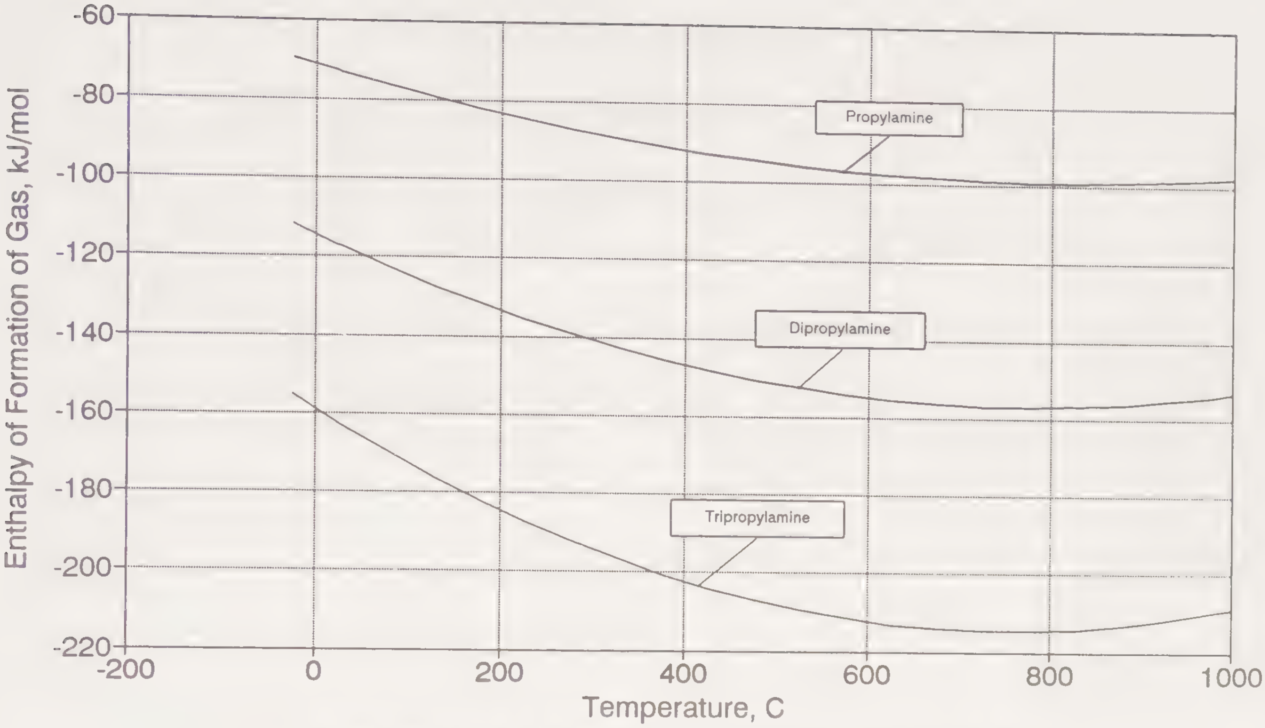

Figure 18-11 Enthalpy of Formation of Gas

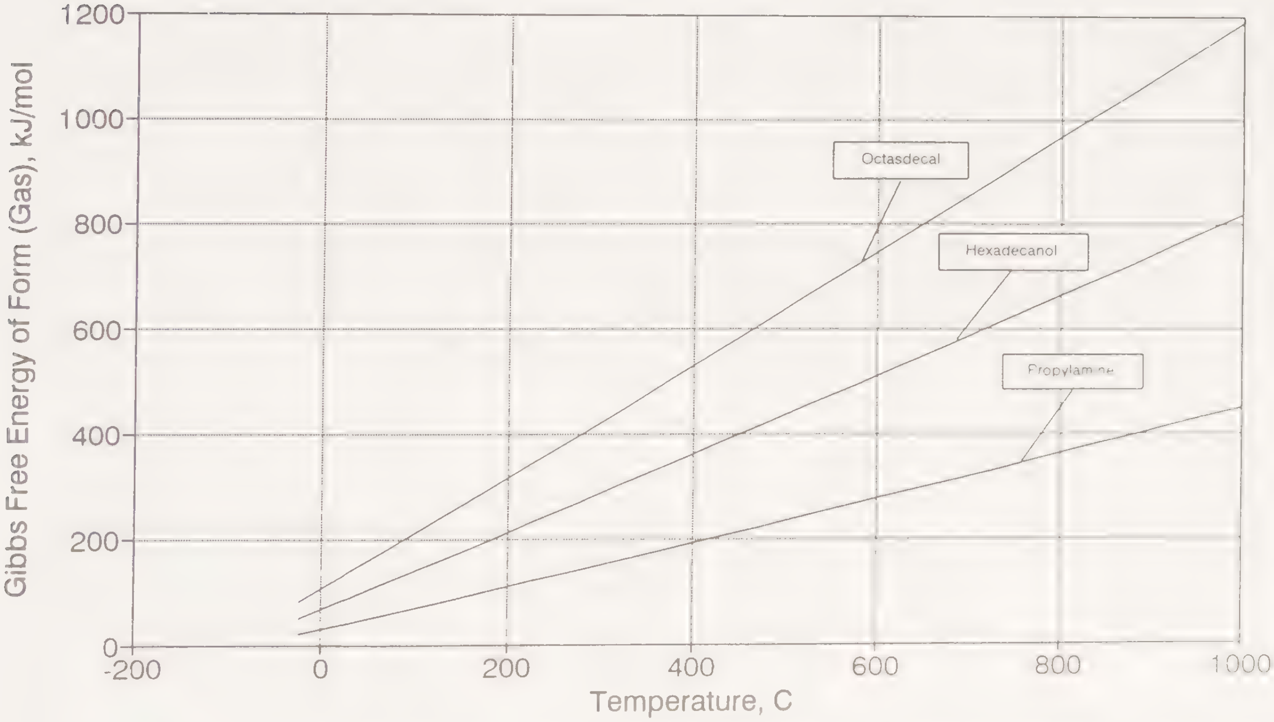

Figure 18-12 Gibbs Free Energy of Formation of Gas

Chapter 19

DIAMINES

Robert W. Gallant and Carl L. Yaws

PHYSICAL PROPERTIES - Table 19-1

Property data from the literature (5,21,25-27,36,63,65,73-75,77,79,82,87,93,103,128-133) are given in Table 19-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 19-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 19-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with possible errors of 5%.

LIQUID DENSITY - Figure 19-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 5% in most cases.

SURFACE TENSION - Figure 19-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 19-5 and 19-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was

accomplished using Equation (1-5a). Results are rough with potential errors of about 25% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in rough agreement with data. Errors are about 25% or less in most cases.

VISCOSITY - Figures 19-7 and 19-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in rough agreement with errors being about 50% or less in most cases.

THERMAL CONDUCTIVITY - Figures 19-9 and 19-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is rough with possible errors of 25% in most cases.

ENTHALPY OF FORMATION - Figure 19-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 19-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 19-1 Physical Properties

1. Name	Ethylenediamine	Hexamethylenediamine
2. Formula	C2H8N	C6H16N2
3. Molecular Weight, g/mol	60.099	116.207
4. Critical Temperature, K	593.00	663.00
5. Critical Pressure, bar	62.9	32.9
6. Critical Volume, ml/mol	264.0	475.0
7. Critical Compressibility Factor	0.337	0.284
8. Acentric Factor	0.4789	0.6501
9. Melting Point, K	284.29	313.95
10. Boiling Point @ 1 atm, K	390.41	475.04
11. Heat of Vaporization @ BP, kJ/kg	665.73	422.05
12. Density of Liquid @ 25 C, g/ml	0.893	0.591 @ BP
13. Surface Tension @ 25 C, dynes/cm	41.88	7.82 @ BP
14. Heat Capacity of Gas @ 25 C, J/g K	1.521	1.583
15. Heat Capacity of Liquid @ 25 C, J/g K	2.87	3.00 @ BP
16. Viscosity of Gas @ 25 C, micropoise	72.15	54.48
17. Viscosity of Liquid @ 25 C, centipoise	1.874	0.170 @ BP
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.013	0.013
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.232	0.103 @ BP
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-17.90	-100.07
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	102.20	136.62
22. Flash Point, K	307.04	366.48
23. Autoignition Temperature, K	658.15	------
24. Lower Explosion Limit in Air, vol %	4.2	0.7
25. Upper Explosion Limit in Air, vol %	14.4	6.3
26. Solubility in Water @ 25 C, ppm(wt)	------	------

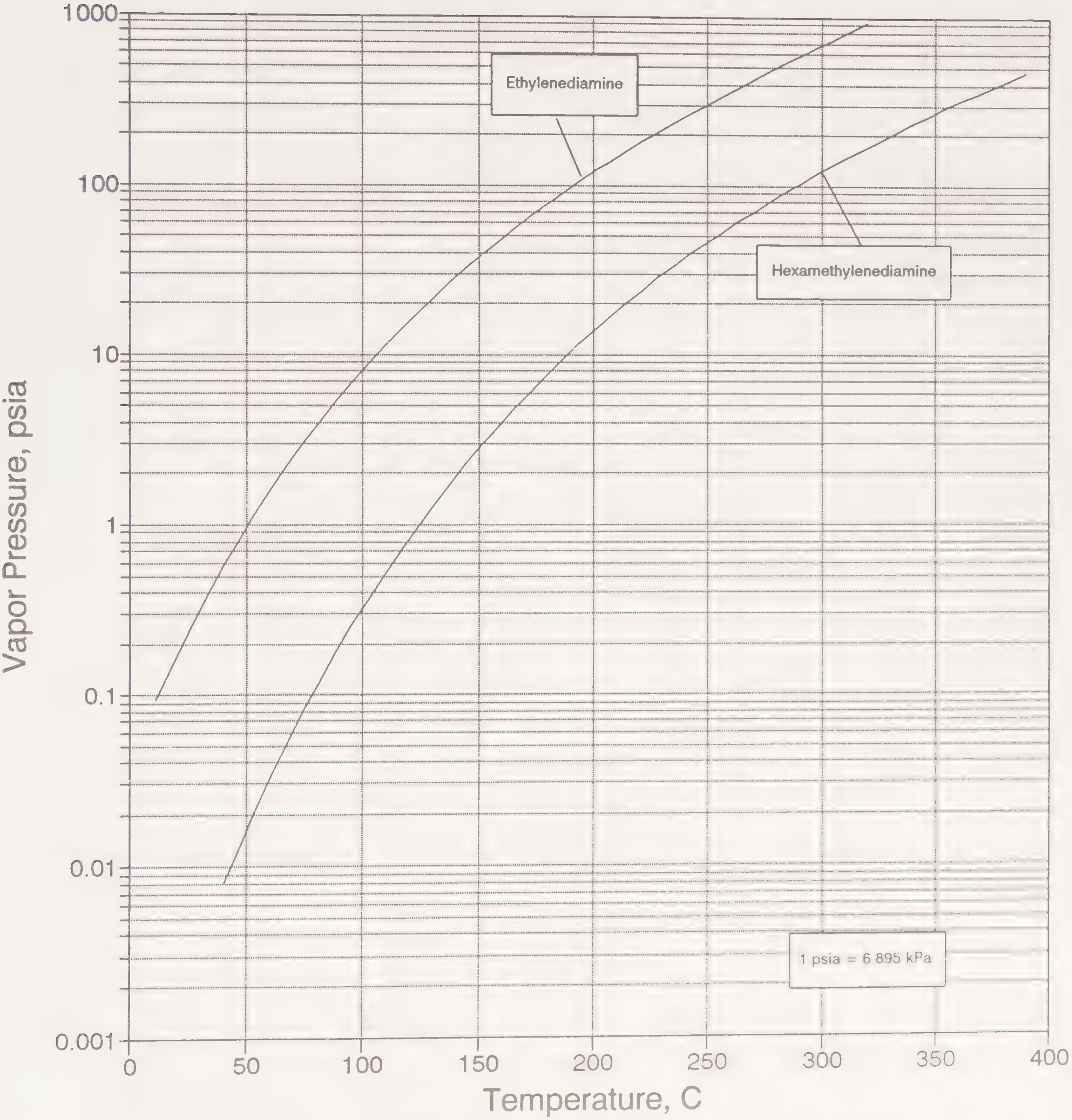

Figure 19-1 Vapor Pressure

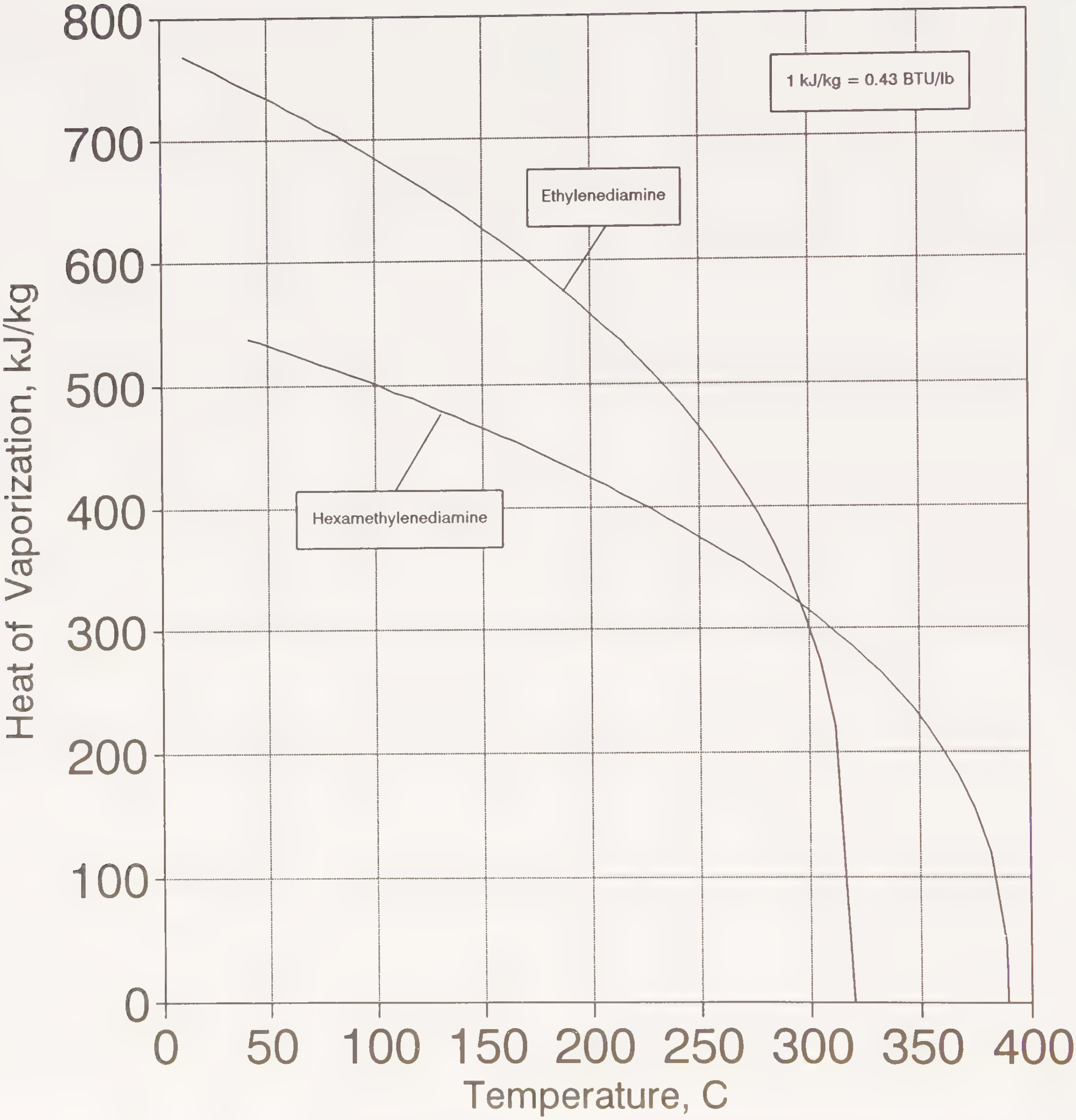

Figure 19-2 Heat of Vaporization

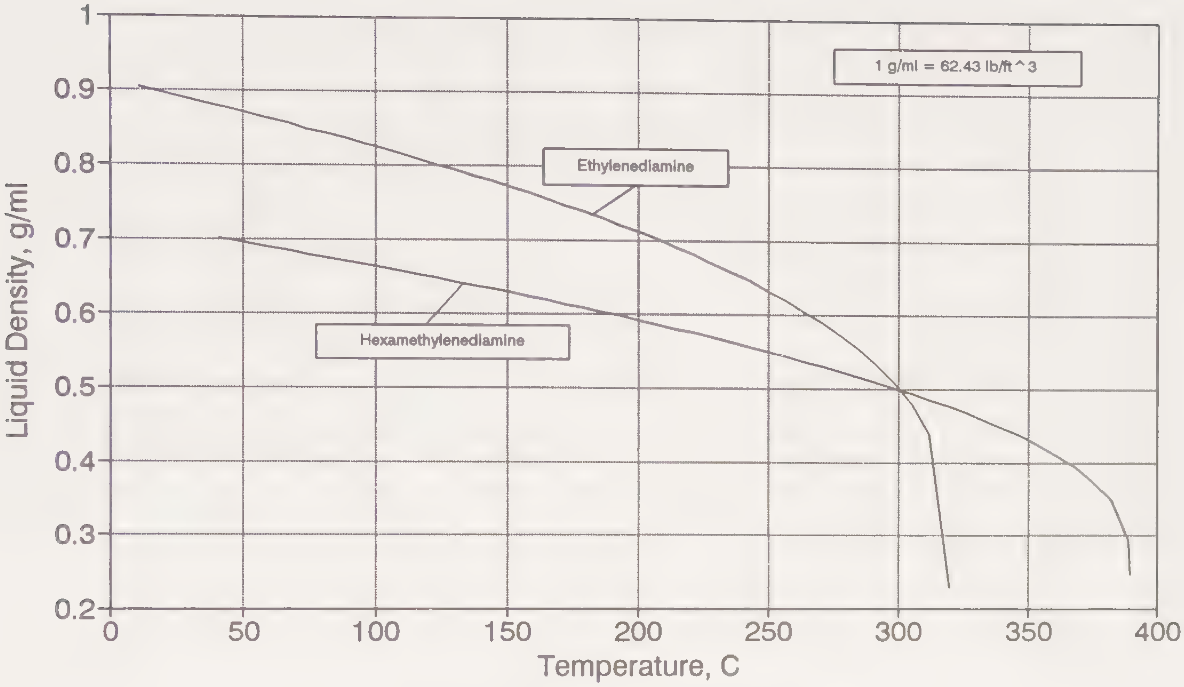

Figure 19-3 Liquid Density

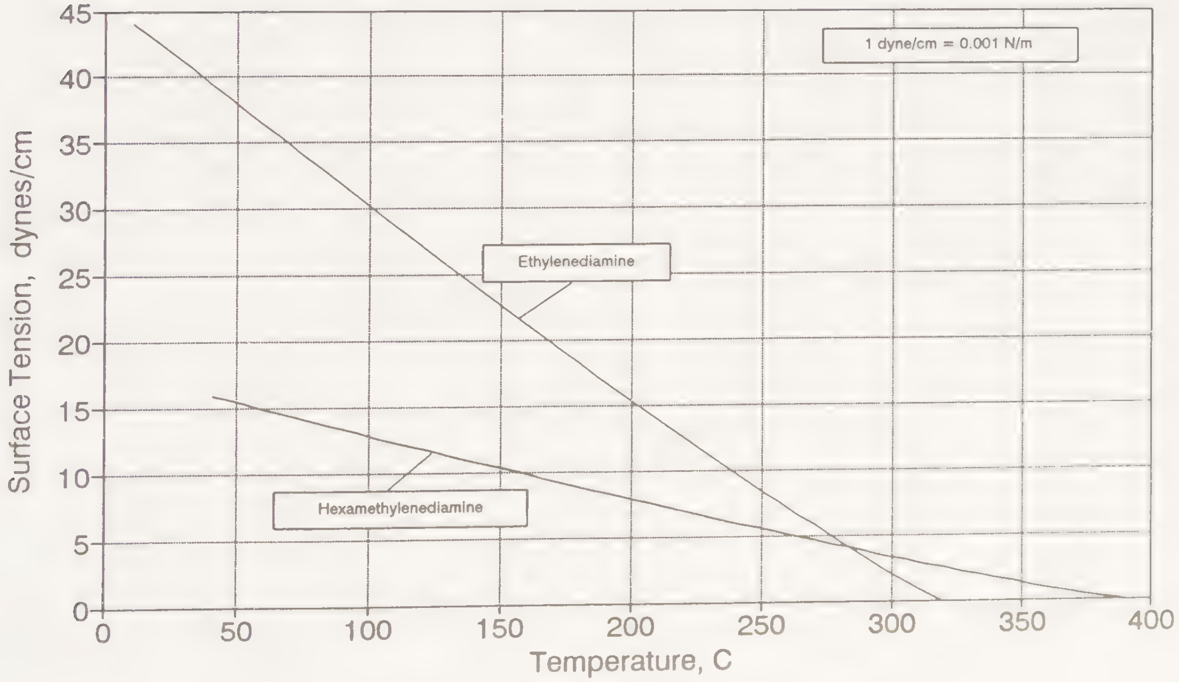

Figure 19-4 Surface Tension

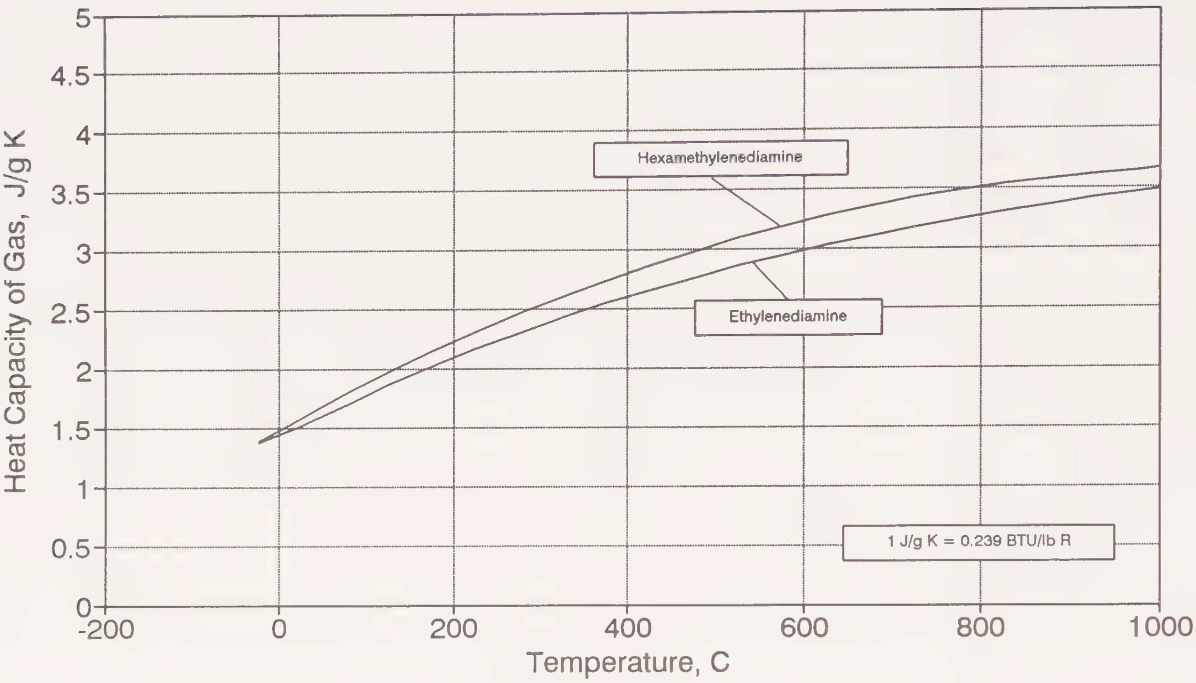

Figure 19-5 Heat Capacity of Gas

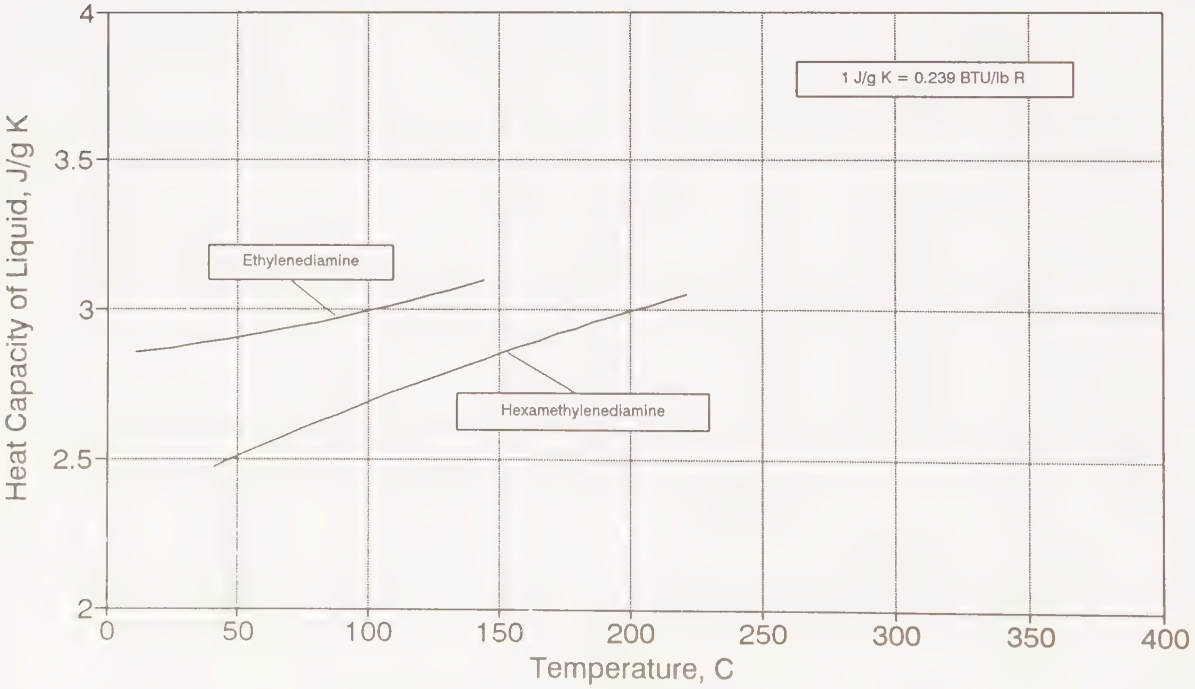

Figure 19-6 Heat Capacity of Liquid

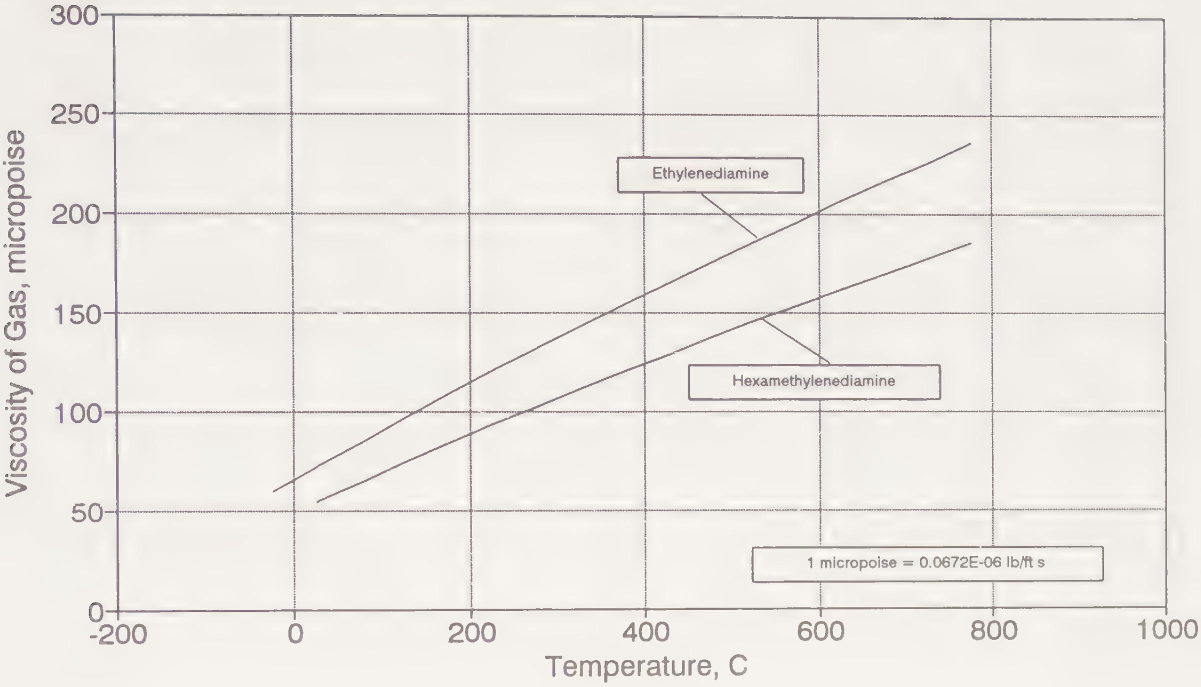

Figure 19-7 Viscosity of Gas

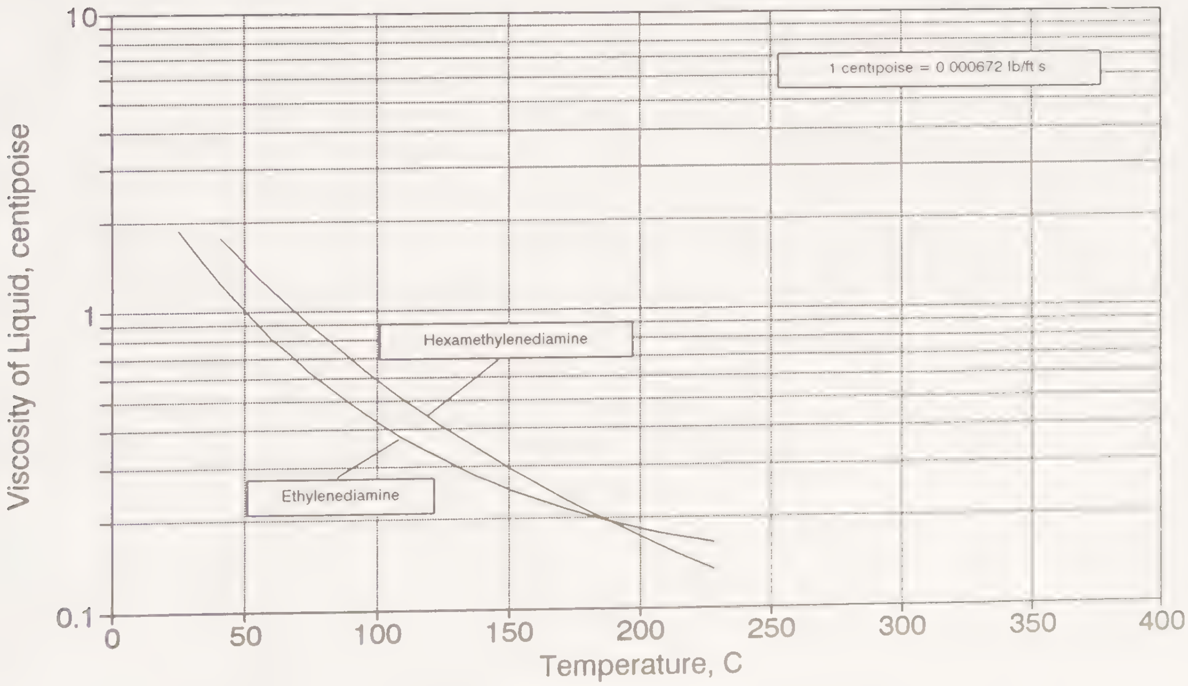

Figure 19-8 Viscosity of Liquid

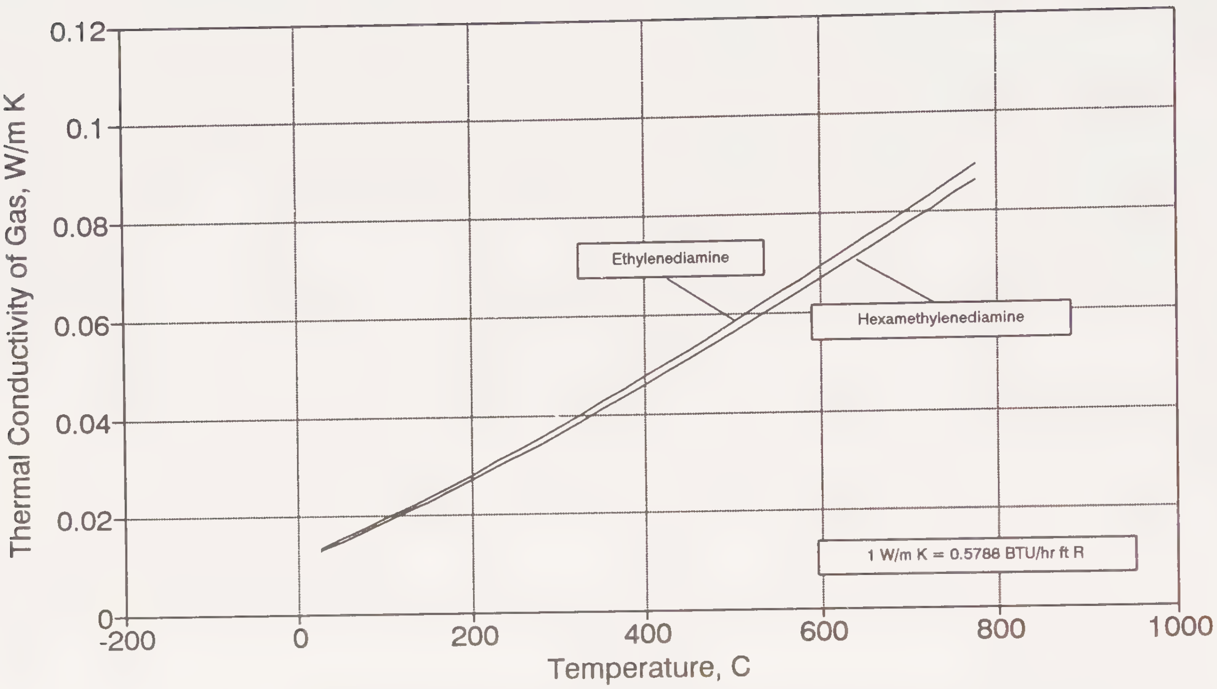

Figure 19-9 Thermal Conductivity of Gas

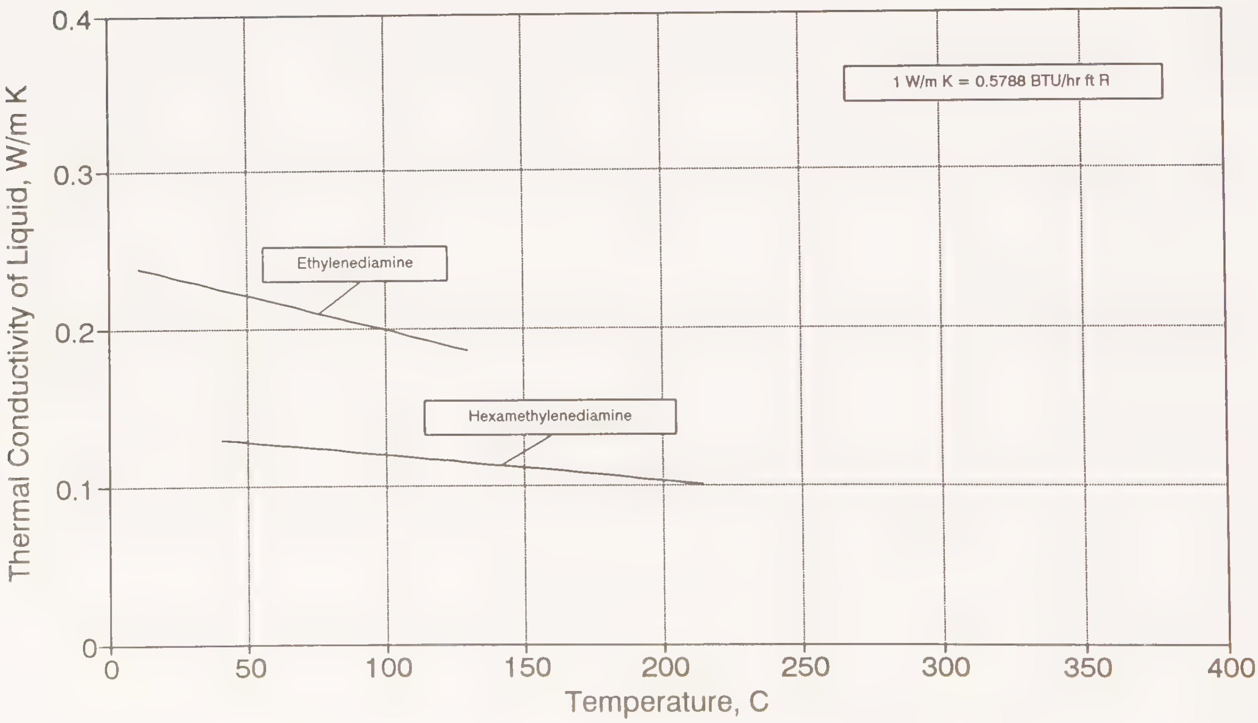

Figure 19-10 Thermal Conductivity of Liquid

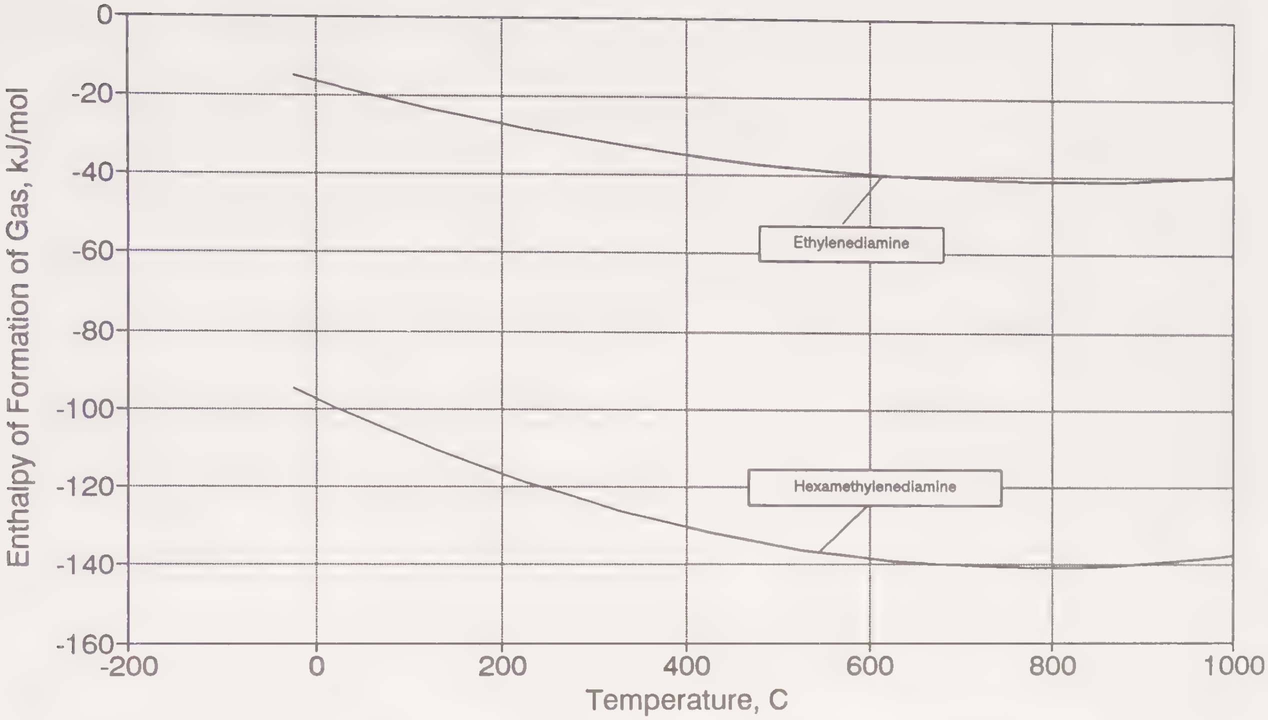

Figure 19-11 Enthalpy of Formation of Gas

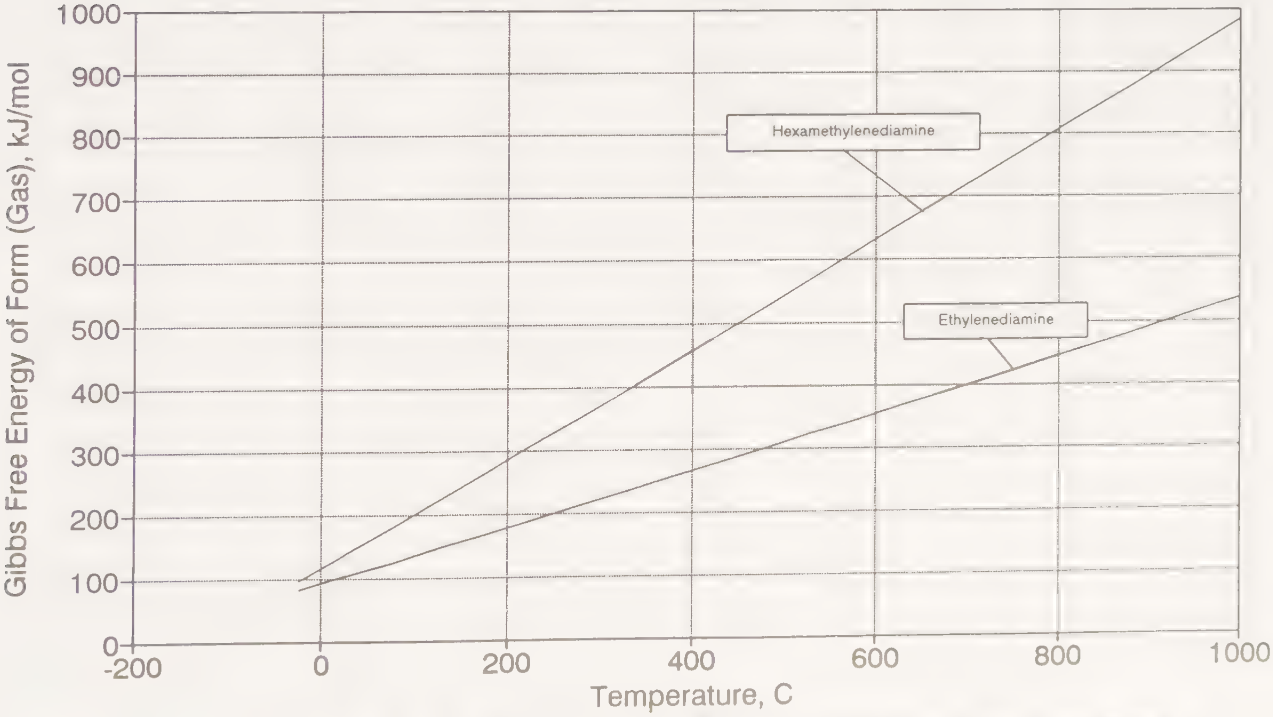

Figure 19-12 Gibbs Free Energy of Formation of Gas

Chapter 20

FORMAMIDES

Robert W. Gallant and Carl L. Yaws

PHYSICAL PROPERTIES - Table 20-1

Property data from the literature (5,8,23,25,26,33,64,73,77,79,82,93,136,138,142-153) are given in Table 20-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available. Several sources (5,26,77) report that formamide slowly decomposes at its boiling point.

VAPOR PRESSURE - Figure 20-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 20-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is favorable with possible errors of 5%.

LIQUID DENSITY - Figure 20-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

SURFACE TENSION - Figure 20-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 20-5 and 20-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was accomplished using Equation (1-5a). Results are favorable with potential errors of about 3% or less in most cases except for N methylformamide (possible 25% error).

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in favorable agreement with data. Errors are about 5% or less in most cases except for N methylformamide (possible 25% error).

VISCOSITY - Figures 20-7 and 20-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases. The curve of formamide was estimated using a similar shape to the curves for N methylformamide and N,N dimethylformamide.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in favorable agreement with errors being about 5% or less in most cases.

THERMAL CONDUCTIVITY - Figures 20-9 and 20-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases. The curve of formamide was estimated using a similar shape to the curves for N methylformamide and N,N dimethylformamide.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 20-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 20-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 20-1 Physical Properties

1. Name	Formamide	N Methyl-formamide	N,N Dimethyl-formamide
2. Formula	CH3NO	C2H5NO	C3H7NO
3. Molecular Weight, g/mol	45.041	59.068	73.095
4. Critical Temperature, K	771.0	721.0	647.0
5. Critical Pressure, bar	78.0	56.2	44.2
6. Critical Volume, ml/mol	163.0	215.0	267.0
7. Critical Compressibility Factor	0.198	0.202	0.219
8. Acentric Factor	0.4534	0.4100	0.3755
9. Melting Point, K	275.7	269.35	212.72
10. Boiling Point @ 1 atm, K	493.0	472.66	426.15
11. Heat of Vaporization @ BP, kJ/kg	1071.32	799.48	539.15
12. Density of Liquid @ 25 C, g/ml	1.129	0.999	0.945
13. Surface Tension @ 25 C, dynes/cm	56.67	38.52	34.43
14. Heat Capacity of Gas @ 25 C, J/g K	1.02	0.98	1.24
15. Heat Capacity of Liquid @ 25 C, J/g K	2.40	2.16	2.06
16. Viscosity of Gas @ 25 C, micropoise	57.44	84.67	61.44
17. Viscosity of Liquid @ 25 C, centipoise	3.347	1.678	0.826
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.0089	0.0100	0.0099
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.353	0.203	0.184
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-186.50	-184.79	-192.22
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-141.55	-109.07	-89.37
22. Flash Point, K	448.15	376.00	330.93
23. Autoignition Temperature, K	------	------	718.15
24. Lower Explosion Limit in Air, vol %	7.0	3.6	2.2
25. Upper Explosion Limit in Air, vol %	29.3	18.6	15.2
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

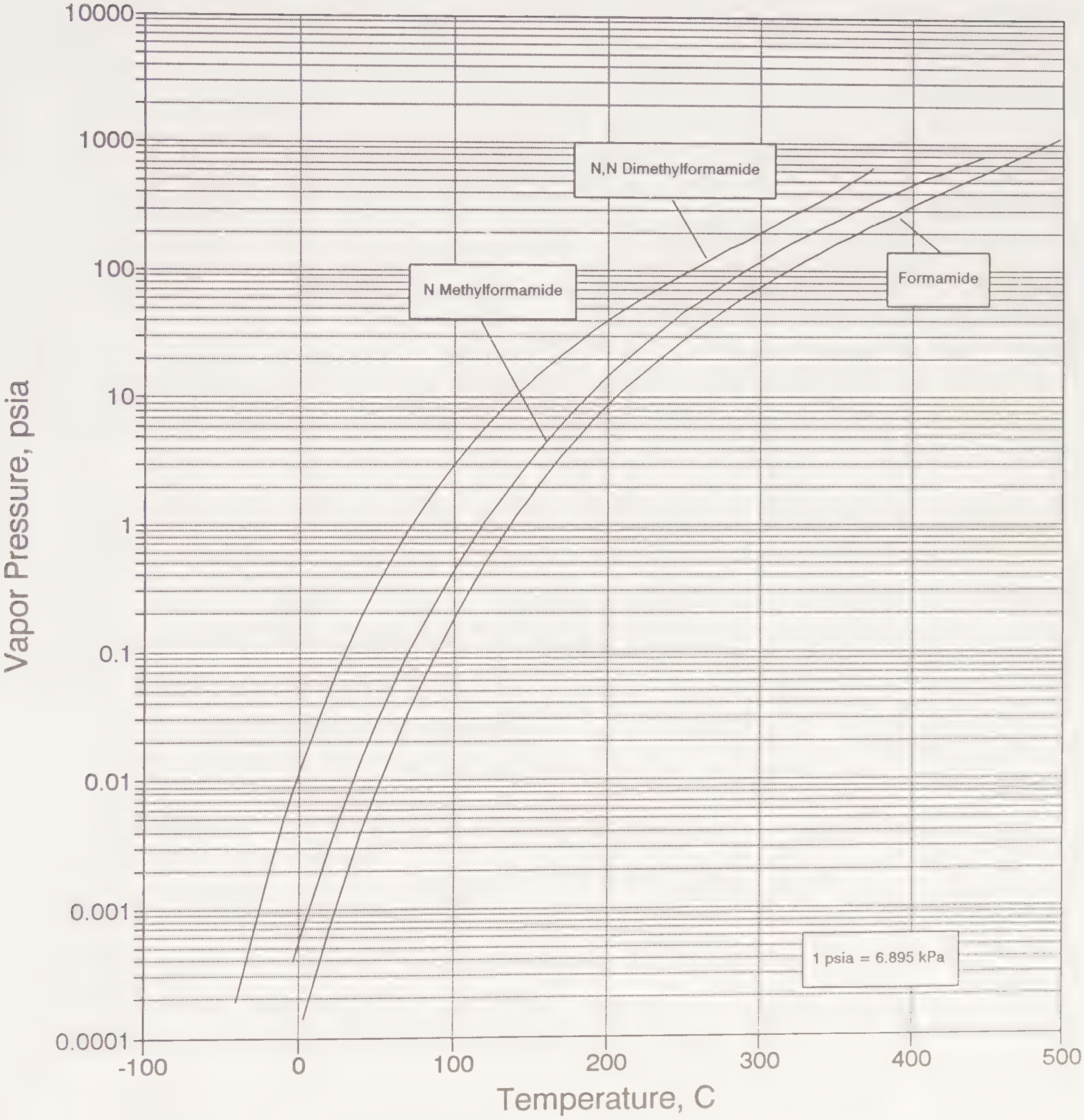

Figure 20-1 Vapor Pressure

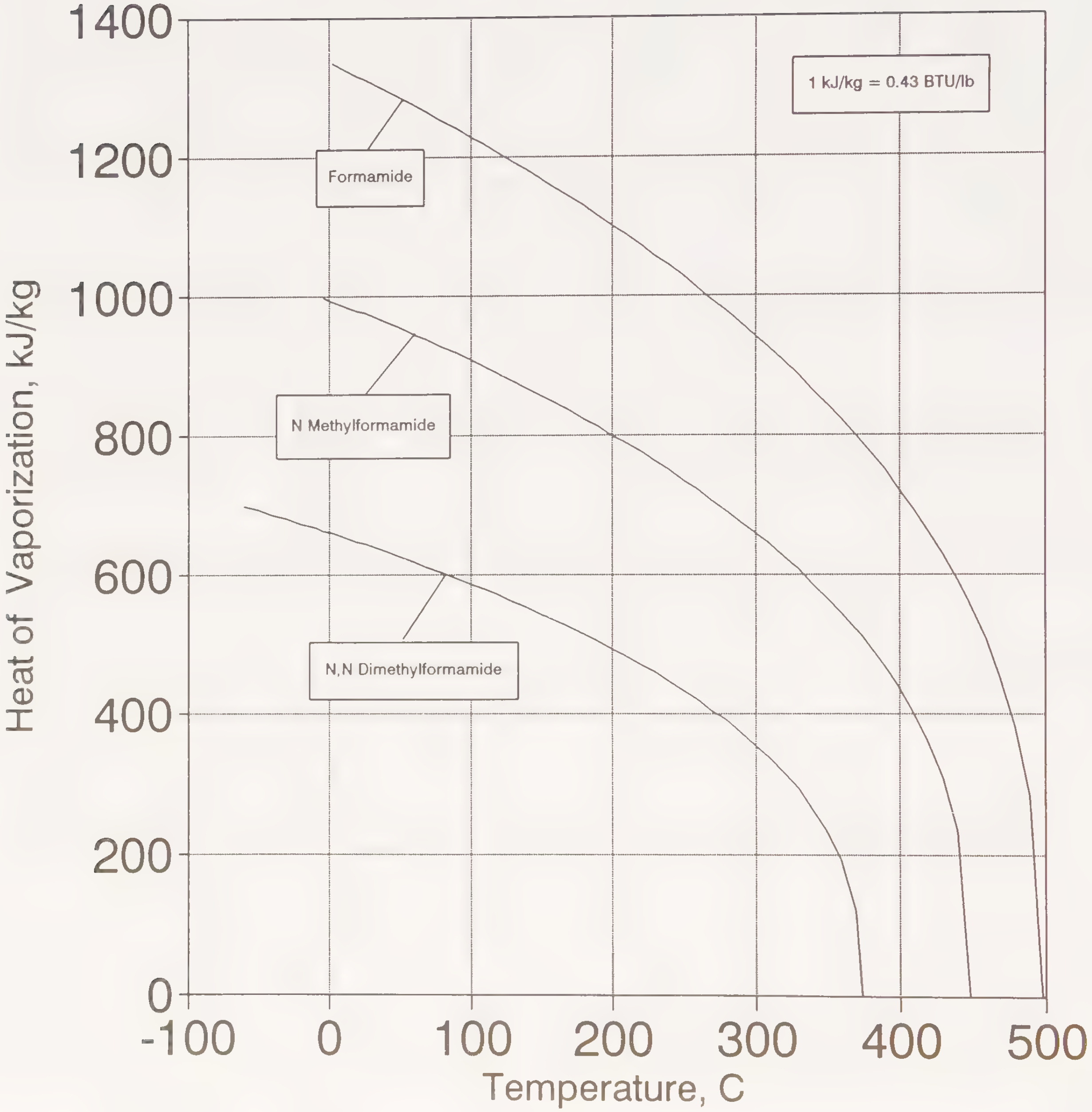

Figure 20-2 Heat of Vaporization

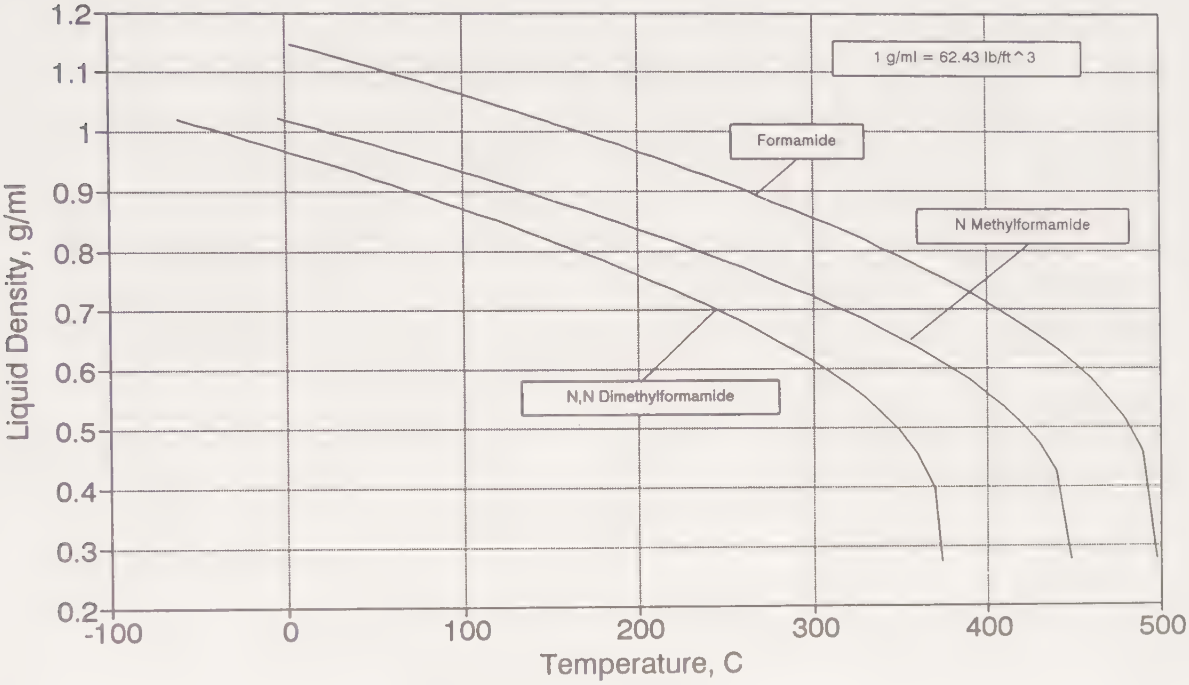

Figure 20-3 Liquid Density

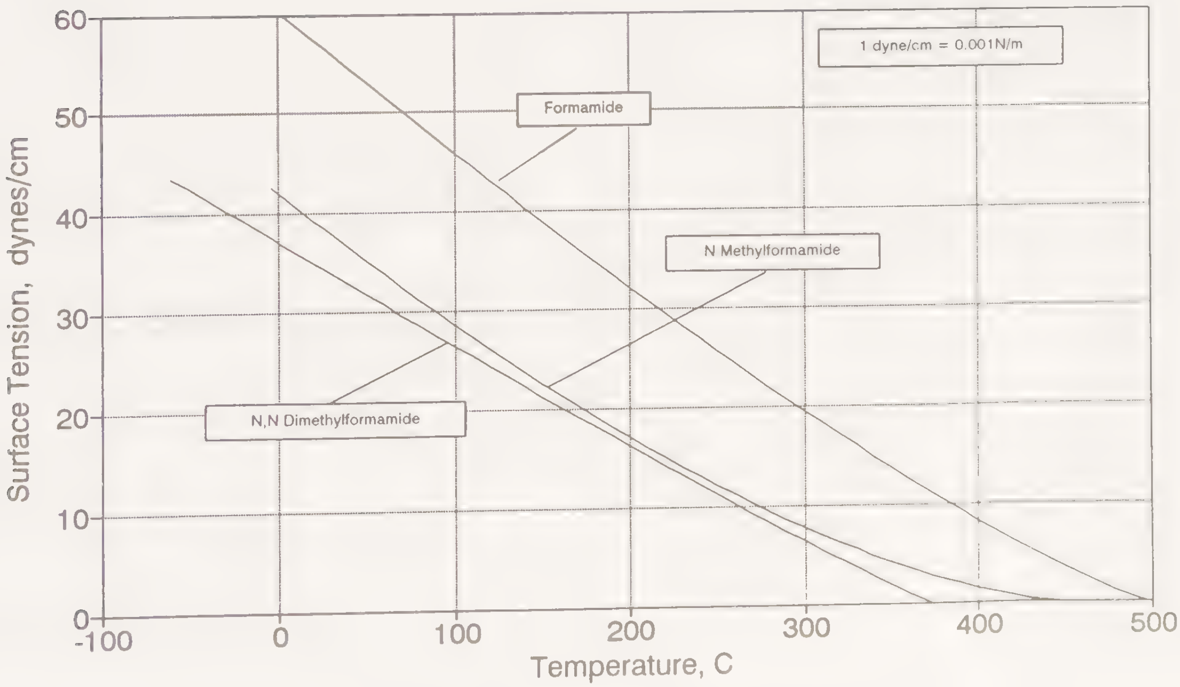

Figure 20-4 Surface Tension

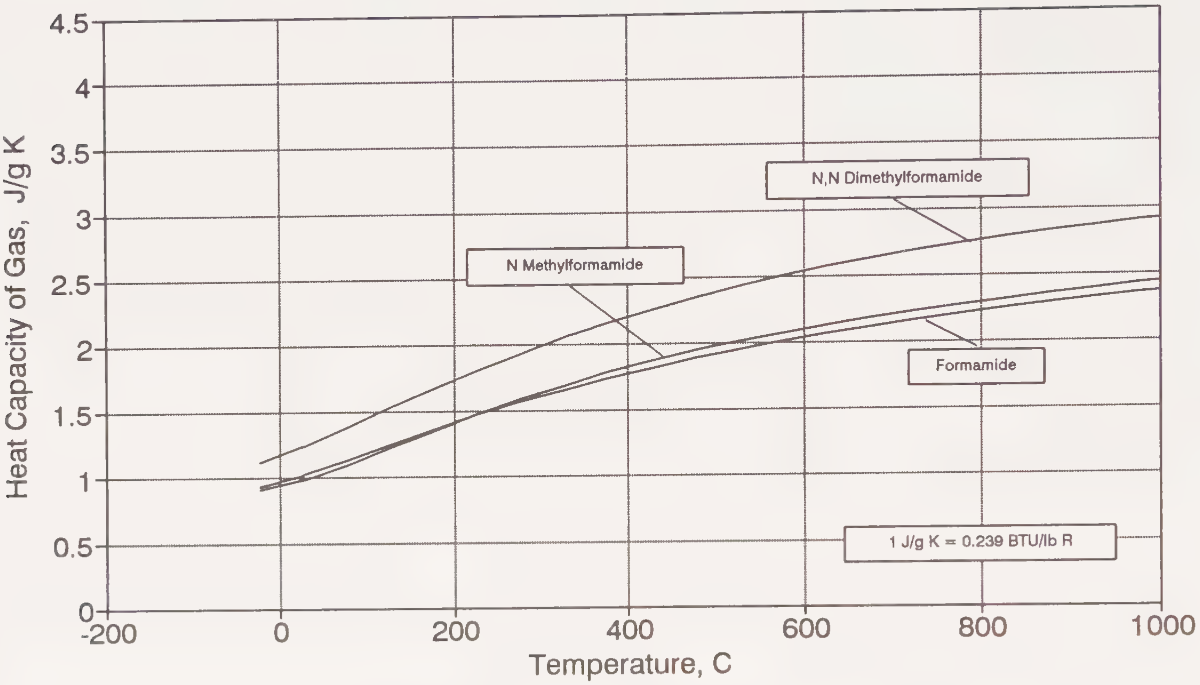

Figure 20-5 Heat Capacity of Gas

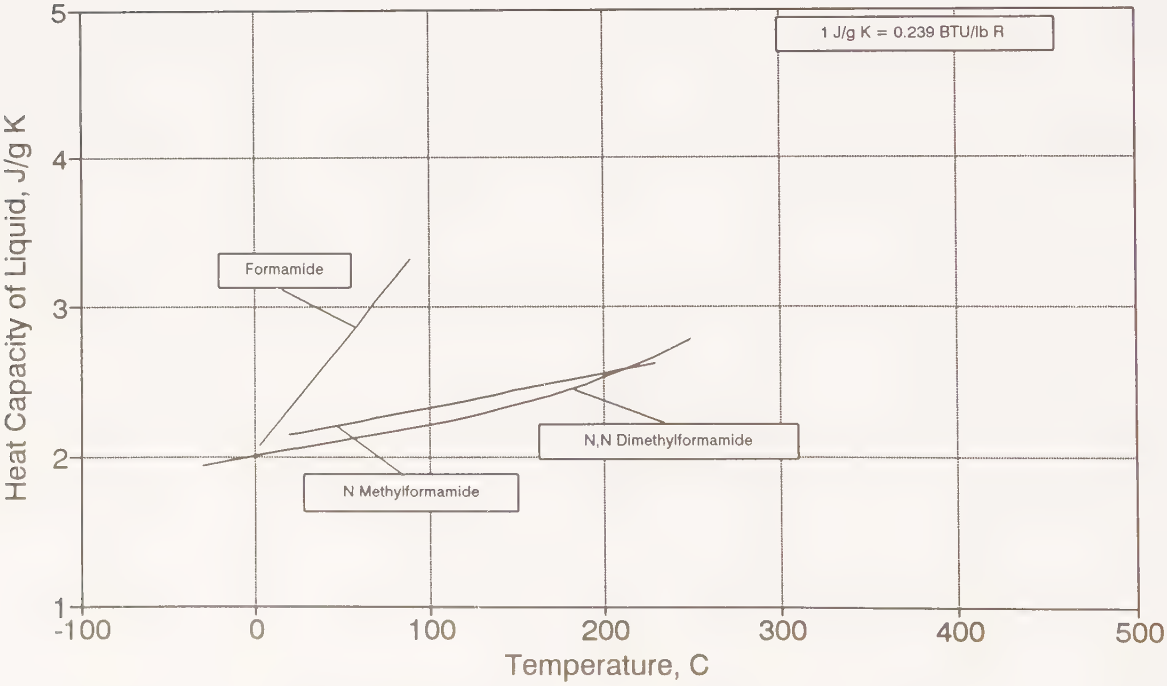

Figure 20-6 Heat Capacity of Liquid

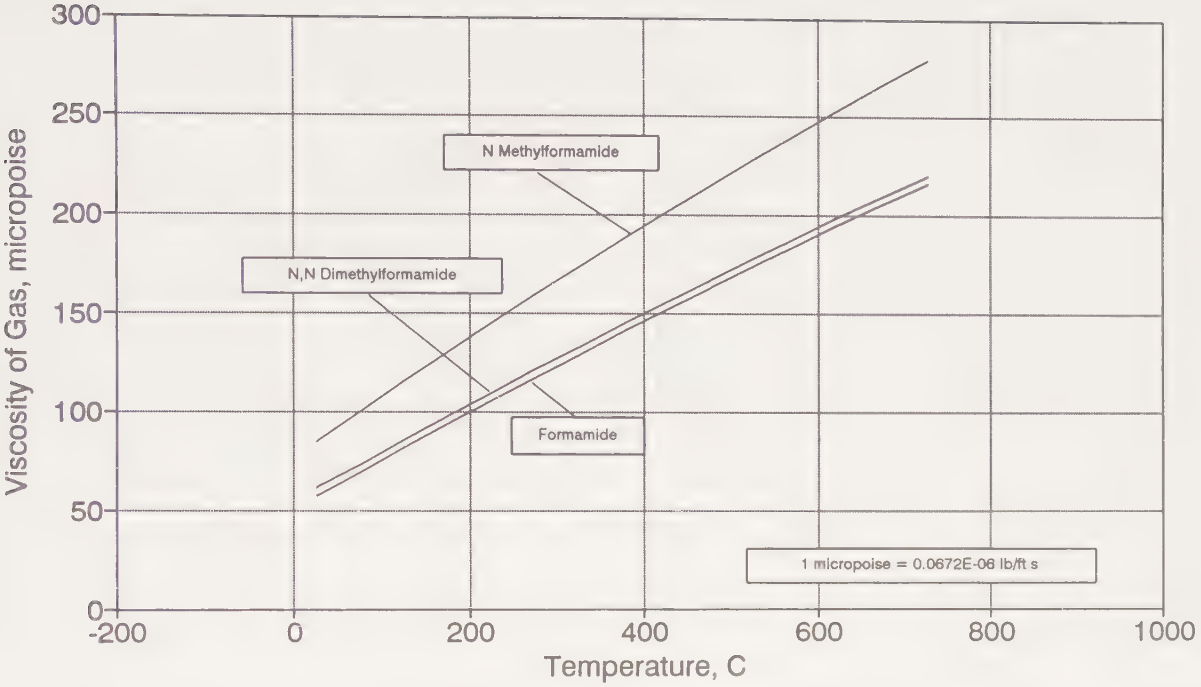

Figure 20-7 Viscosity of Gas

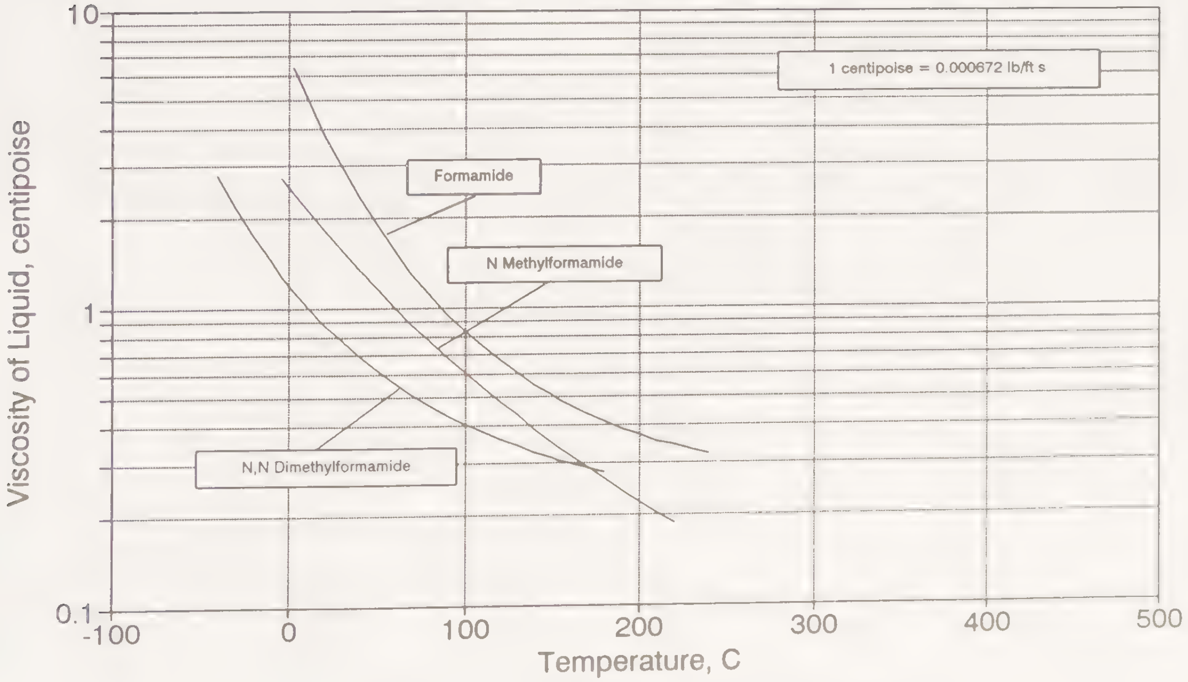

Figure 20-8 Viscosity of Liquid

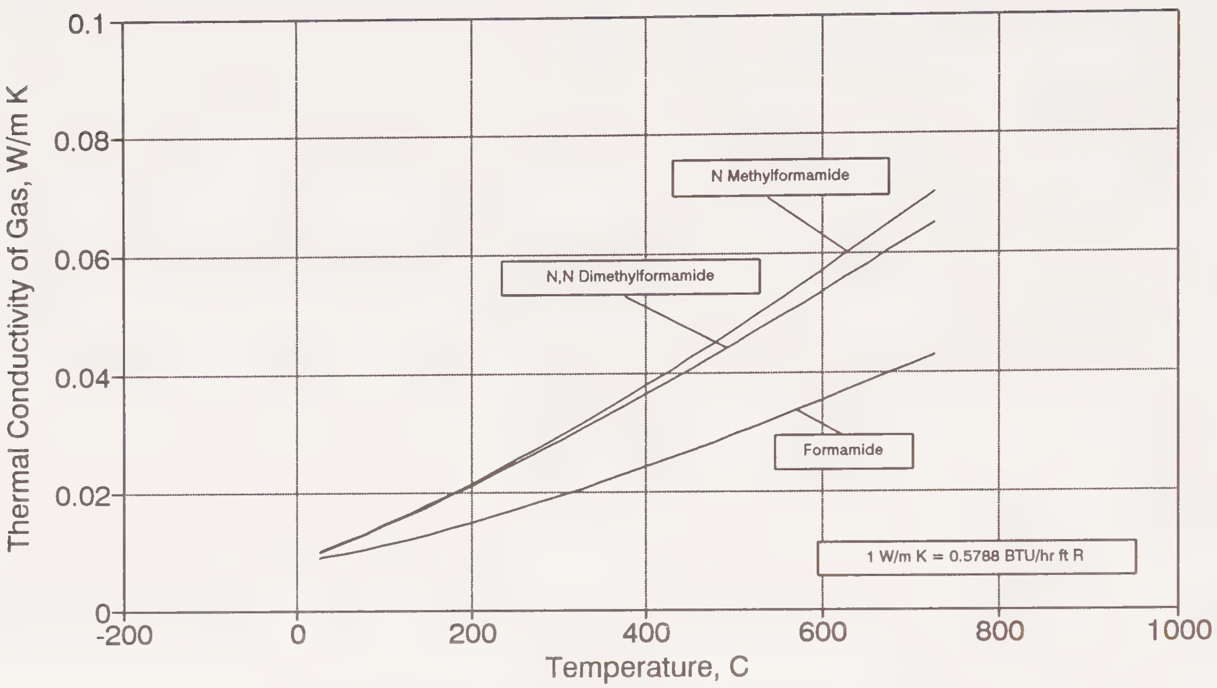

Figure 20-9 Thermal Conductivity of Gas

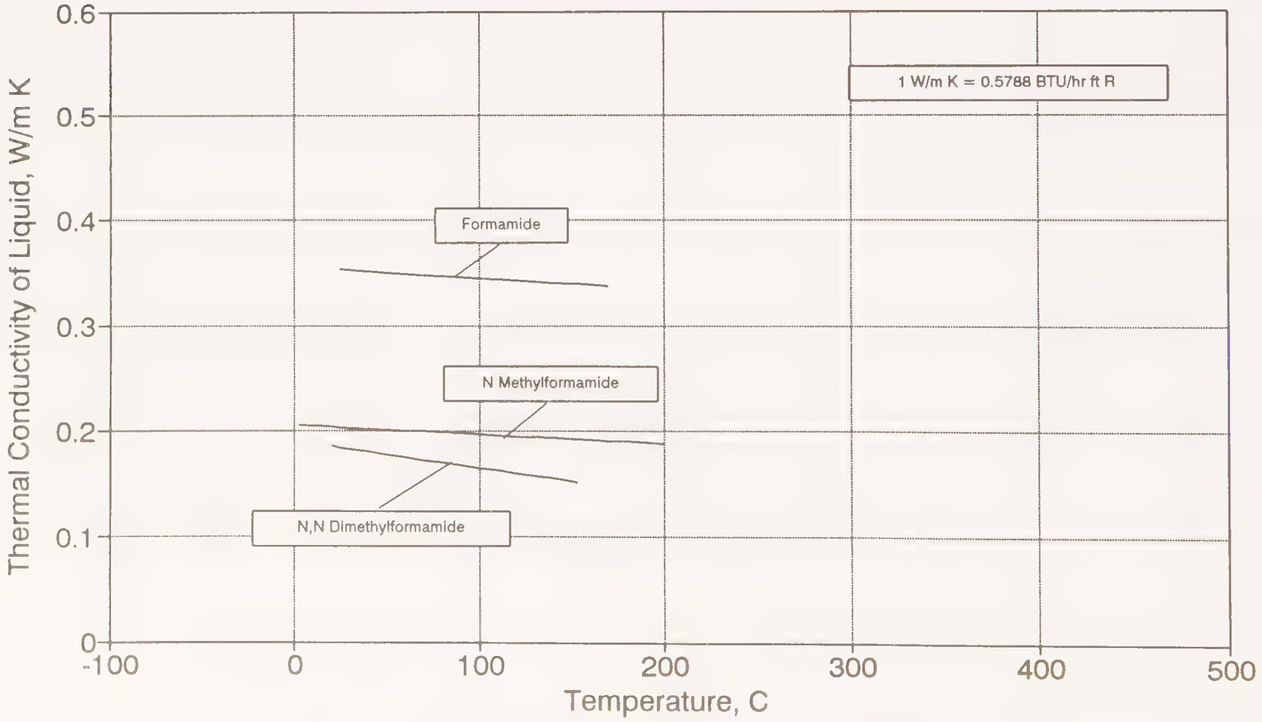

Figure 20-10 Thermal Conductivity of Liquid

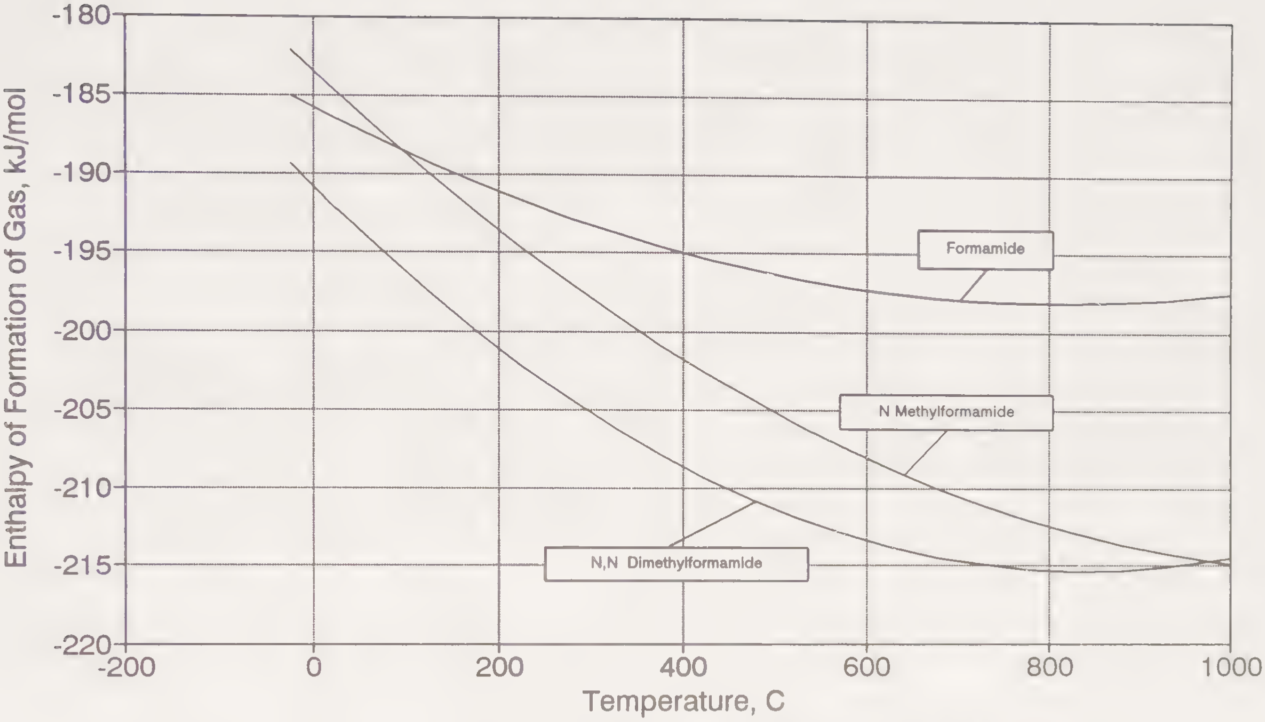

Figure 20-11 Enthalpy of Formation of Gas

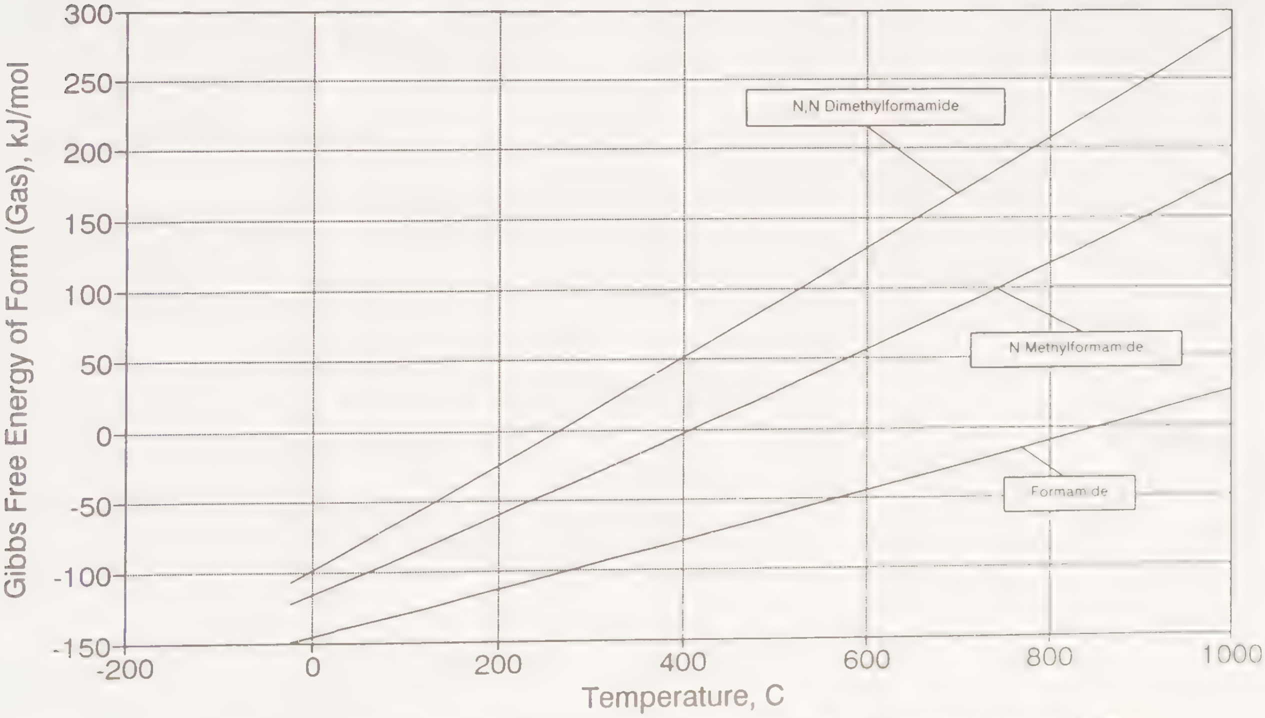

Figure 20-12 Gibbs Free Energy of Formation of Gas

Chapter 21

ACETAMIDES

Robert W. Gallant and Carl L. Yaws

PHYSICAL PROPERTIES - Table 21-1

Property data from the literature (5,8,14,21,25,26,36,62,65,68,73-75,77,87,93,97,99,101,134-141) are given in Table 21-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 21-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in fair agreement with experimental data. Errors are about 10% or less in most cases.

HEAT OF VAPORIZATION - Figure 21-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is fair with possible errors of 10%.

LIQUID DENSITY - Figure 21-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 5% in most cases.

SURFACE TENSION - Figure 21-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 5% or less in most cases.

HEAT CAPACITY - Figures 21-5 and 21-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was

accomplished using Equation (1-5a). Results are fair with potential errors of about 10% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in rough agreement with data. Errors are about 25% or less in most cases.

VISCOSITY - Figures 21-7 and 21-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 10% or less in most cases.

THERMAL CONDUCTIVITY - Figures 21-9 and 21-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is rough with errors less then 25% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 21-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 21-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 21-1 Physical Properties

1. Name	Acetamide	N Methyl-acetamide	N,N Dimethyl-acetamide
2. Formula	C2H5NO	C3H7NO	C4H9NO
3. Molecular Weight, g/mol	59.068	73.095	87.122
4. Critical Temperature, K	761.0	718.0	658.0
5. Critical Pressure, bar	66.0	49.8	40.3
6. Critical Volume, ml/mol	215.0	267.0	321.0
7. Critical Compressibility Factor	0.224	0.223	0.236
8. Acentric Factor	0.3807	0.4351	0.3635
9. Melting Point, K	354.15	301.15	253.15
10. Boiling Point @ 1 atm, K	494.30	478.15	439.25
11. Heat of Vaporization @ BP, kJ/kg	941.42	654.99	466.50
12. Density of Liquid @ BP, g/ml	0.867	0.798	0.801
13. Surface Tension @ BP, dynes/cm	22.93	14.15	15.63
14. Heat Capacity of Gas @ 25 C, J/g K	1.06	1.05	1.27
15. Heat Capacity of Liquid @ BP, J/g K	2.81	2.45	2.10
16. Viscosity of Gas @ 25 C, micropoise	55.68	76.33	59.10
17. Viscosity of Liquid @ BP, centipoise	0.283	0.239	0.211
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.0079	0.0105	0.0087
19. Thermal Conductivity of Liquid @ BP, W/m K	0.171	0.124	0.111
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	-238.86	-240.39	-225.66
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	-160.34	-136.18	-89.79
22. Flash Point, K	399.0	381.15	336.15
23. Autoignition Temperture, K	------	------	627.15
24. Lower Explosion Limit in Air, vol %	3.6	2.4	1.8
25. Upper Explosion Limit in Air, vol %	20.5	13.9	13.8
26. Solubility in Water @ 25 C, ppm(wt)	------	------	------

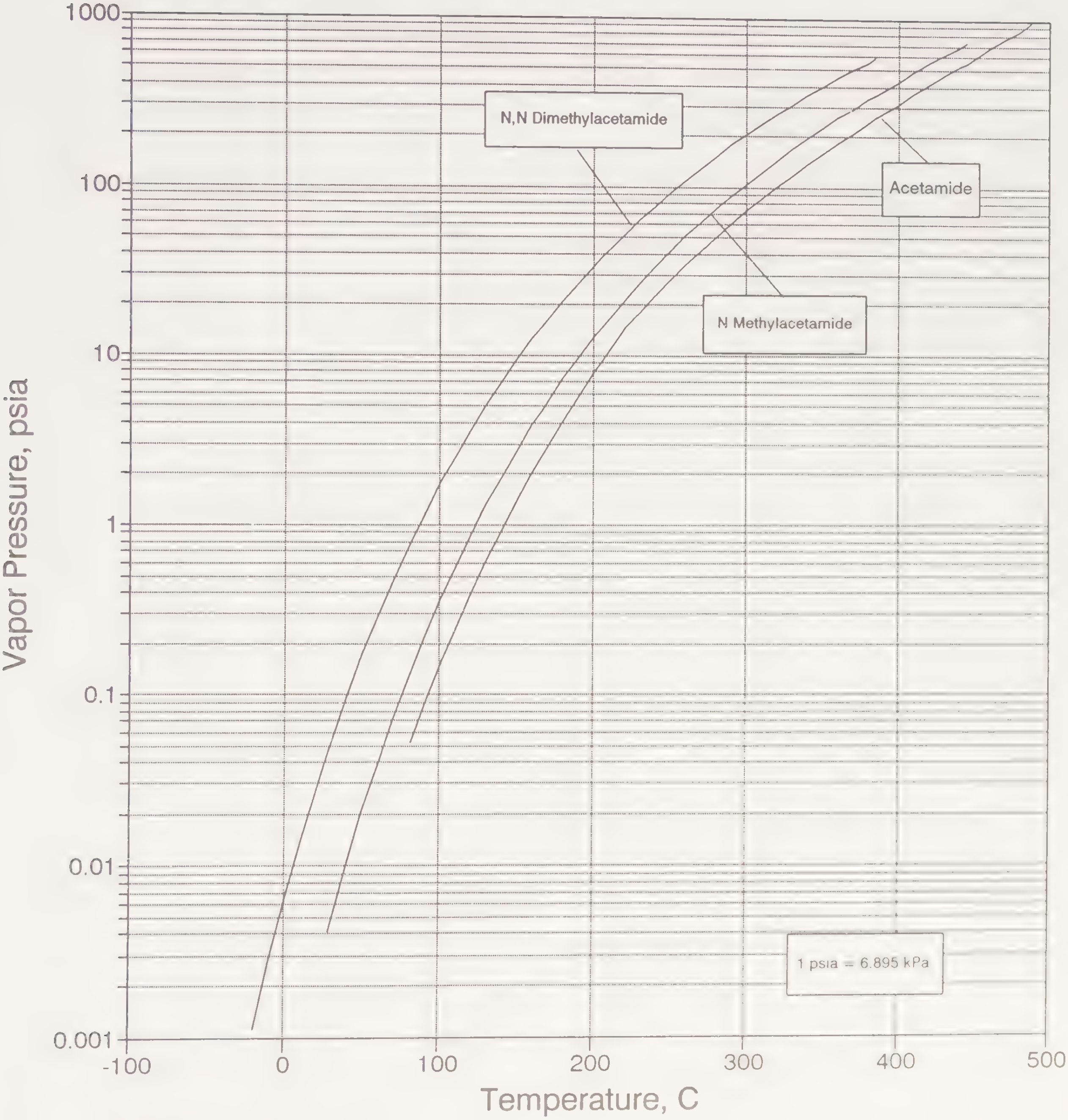

Figure 21-1 Vapor Pressure

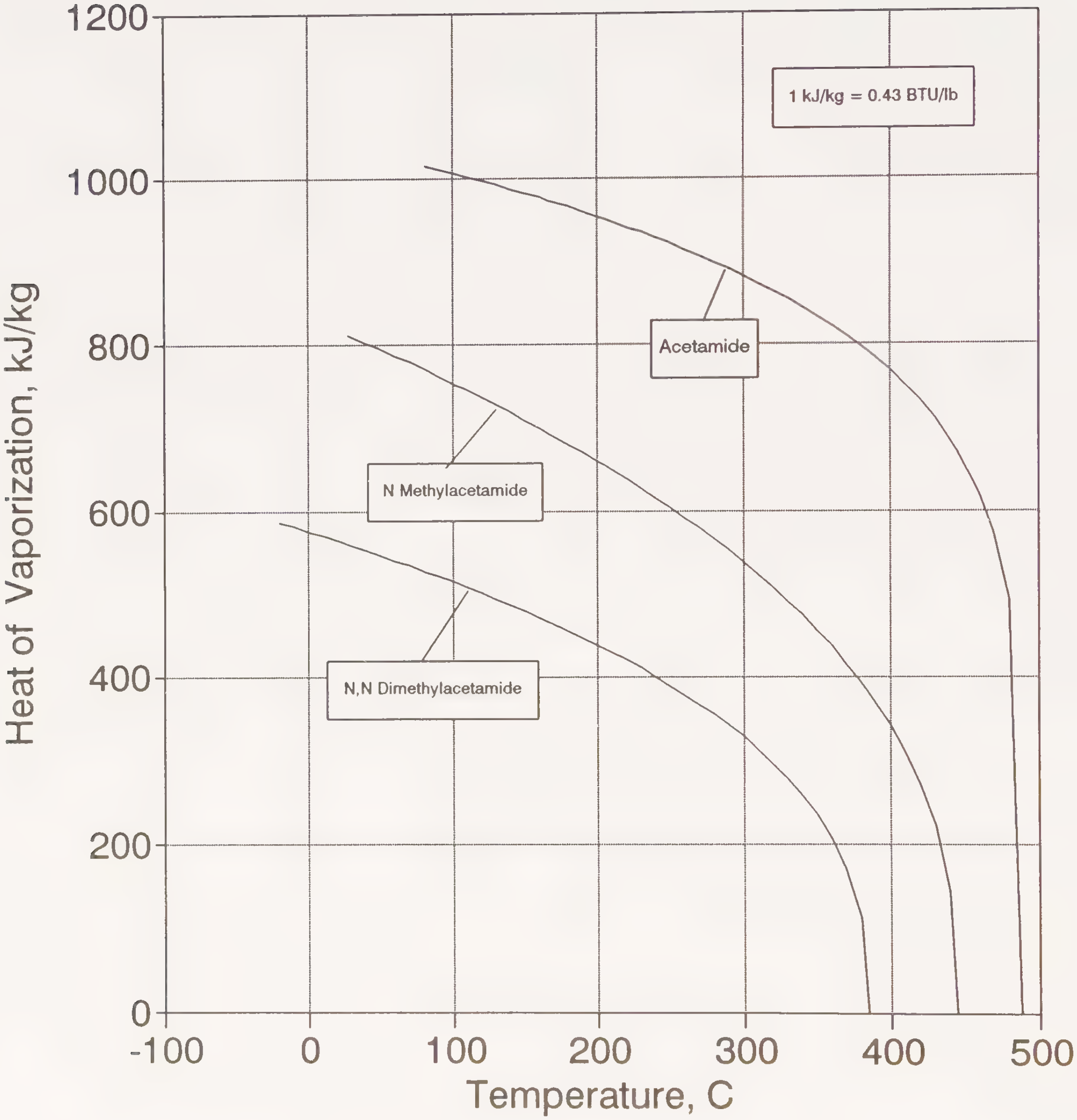

Figure 21-2 Heat of Vaporization

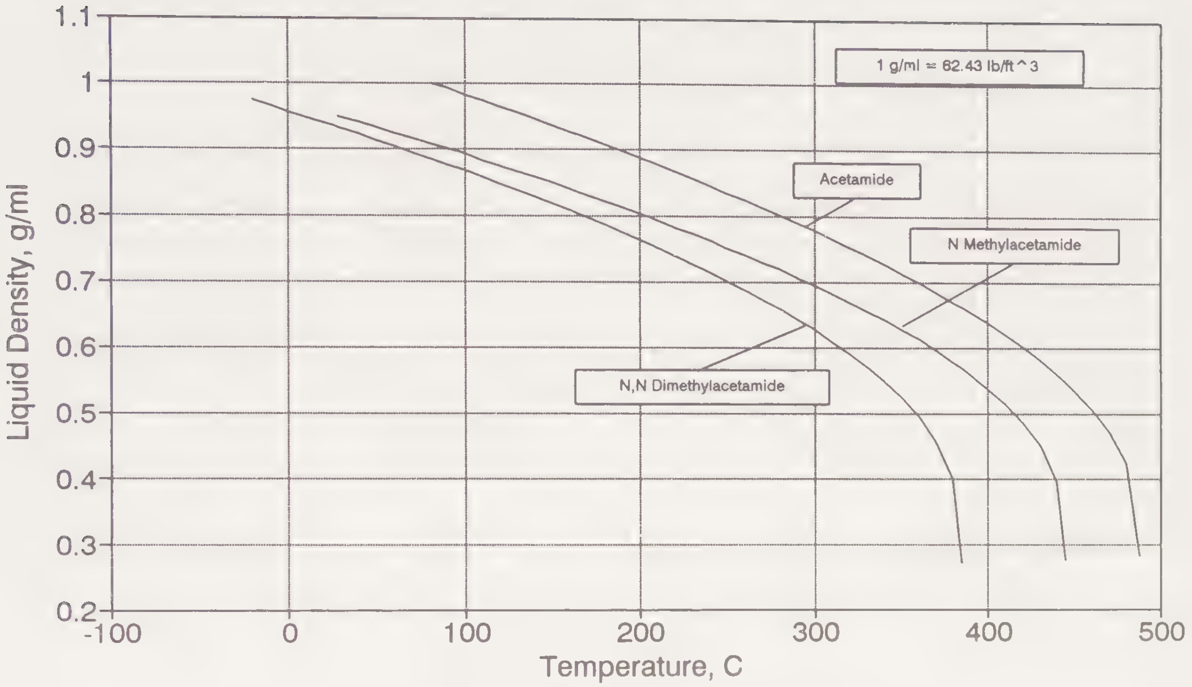

Figure 21-3 Liquid Density

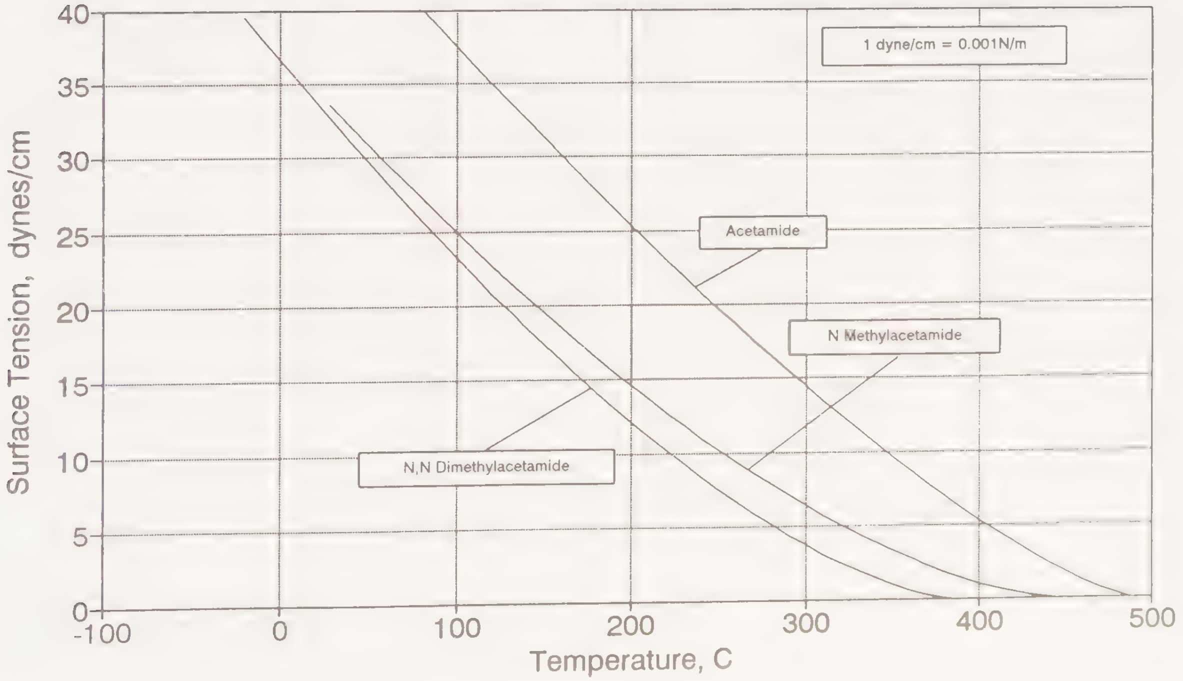

Figure 21-4 Surface Tension

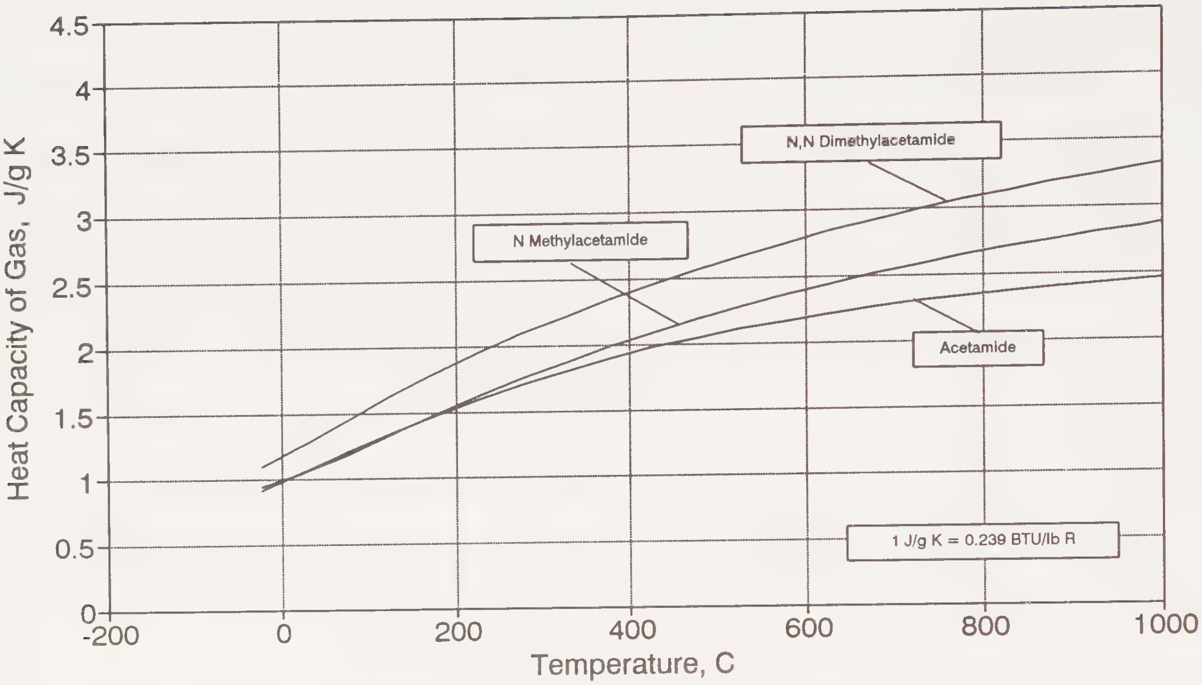

Figure 21-5 Heat Capacity of Gas

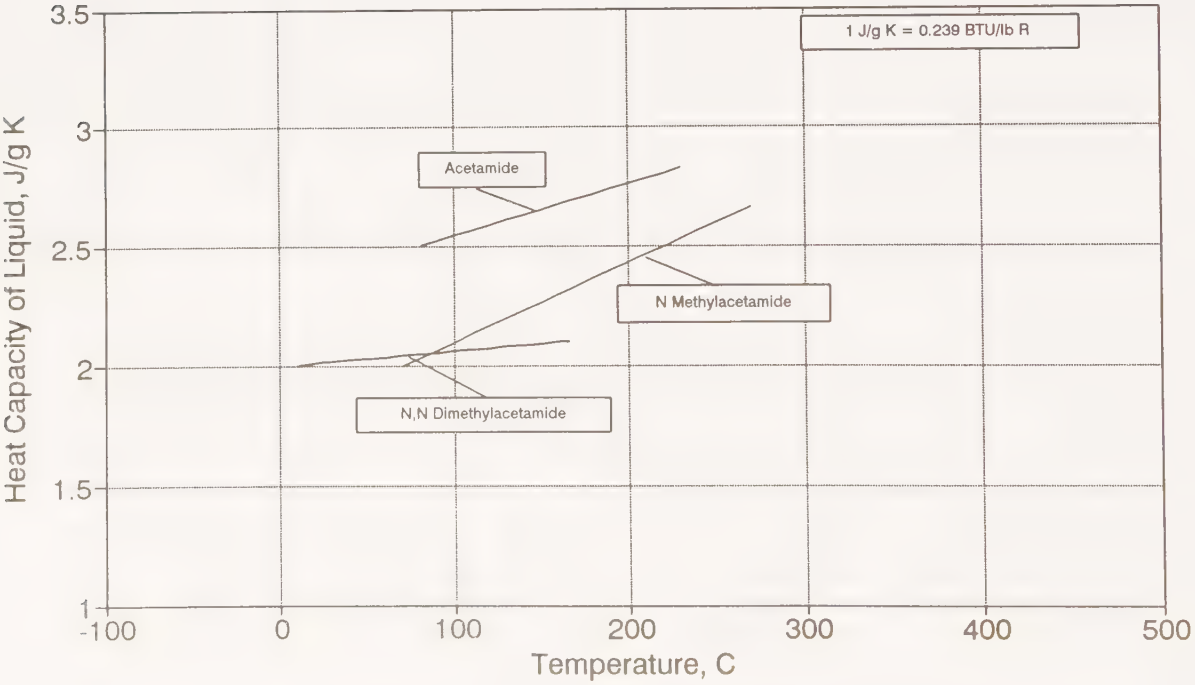

Figure 21-6 Heat Capacity of Liquid

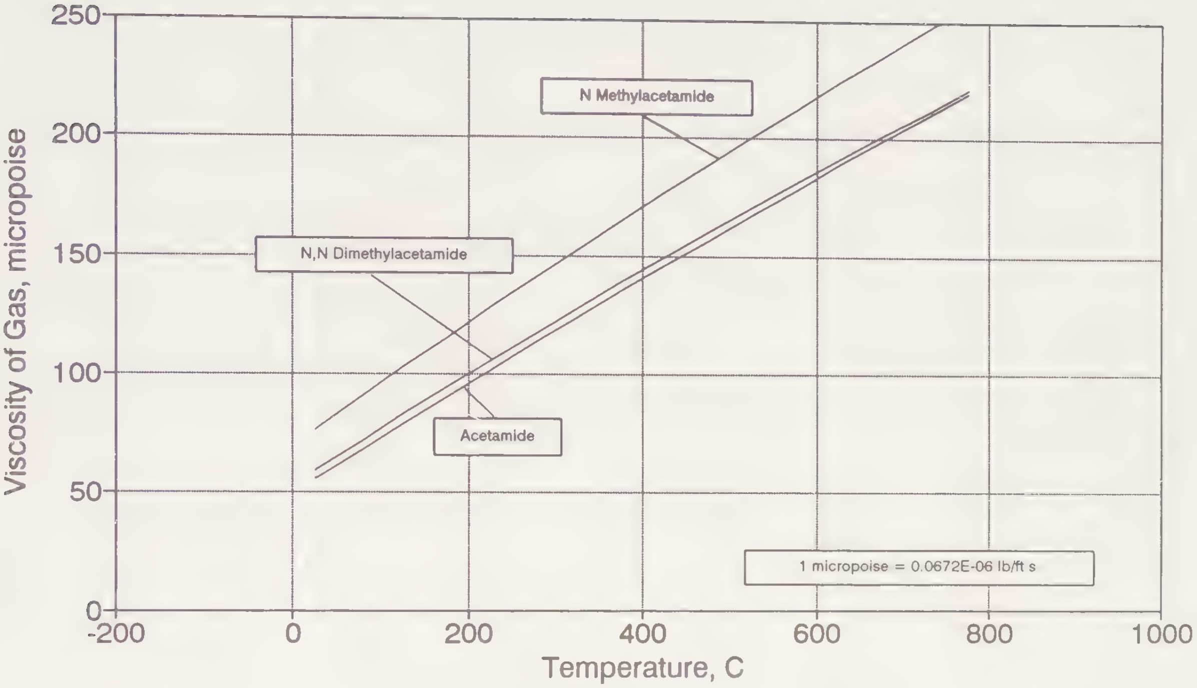

Figure 21-7 Viscosity of Gas

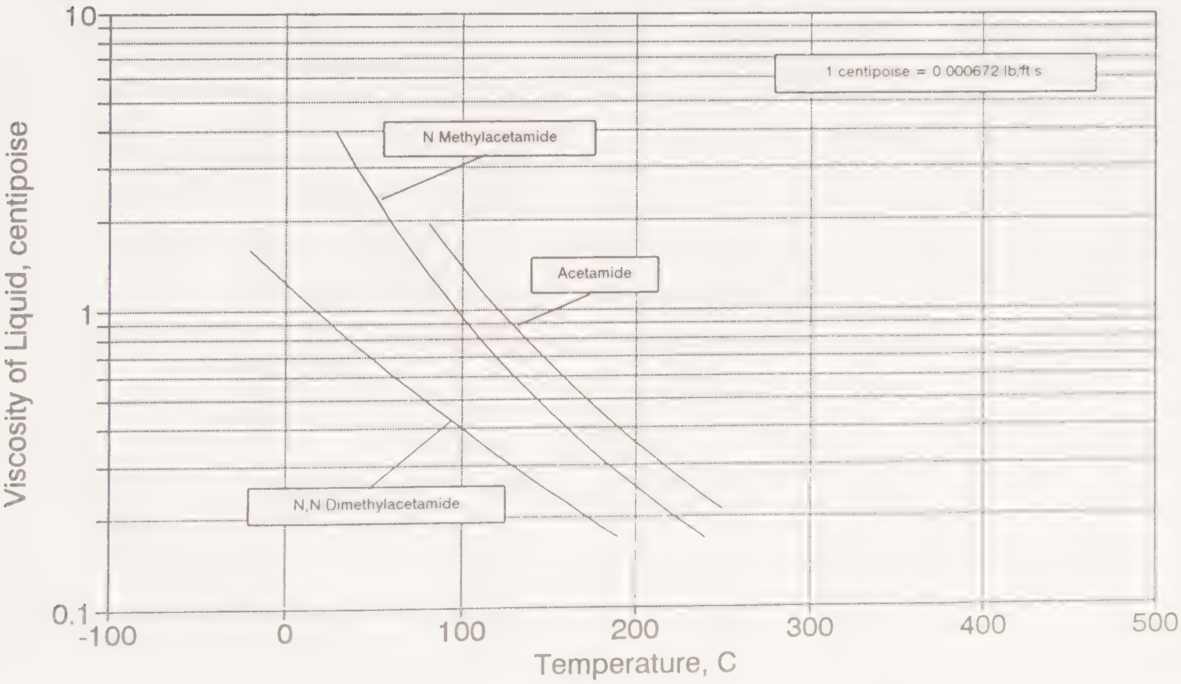

Figure 21-8 Viscosity of Liquid

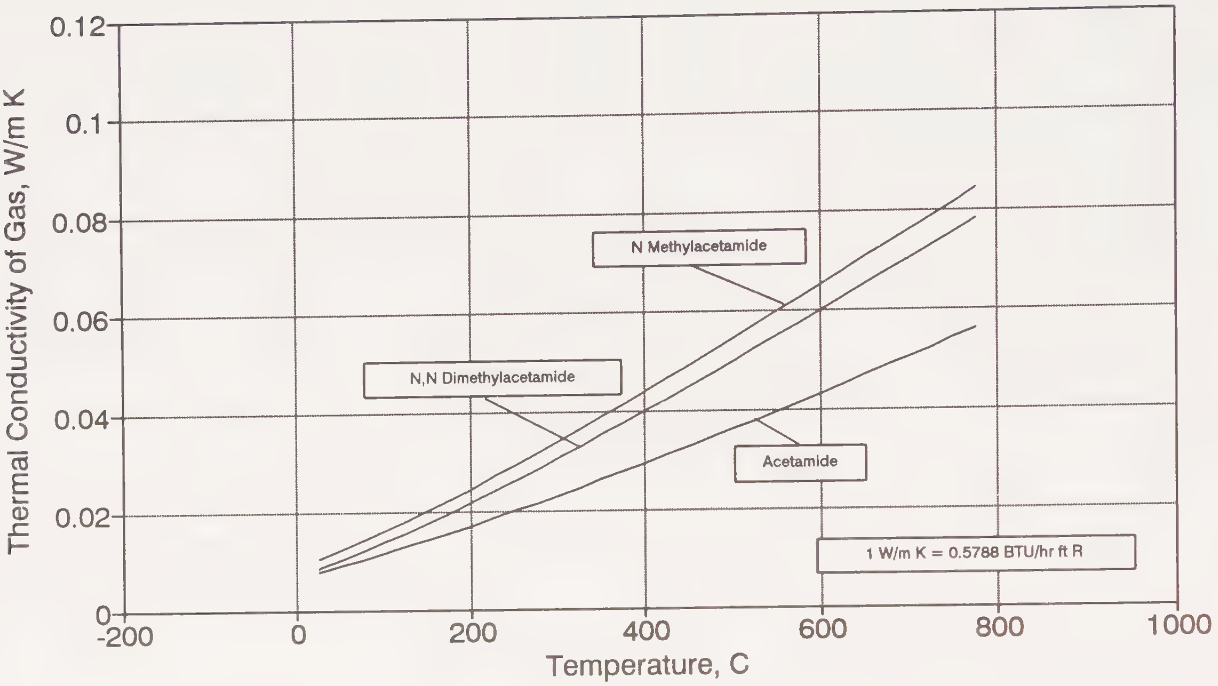

Figure 21-9 Thermal Conductivity of Gas

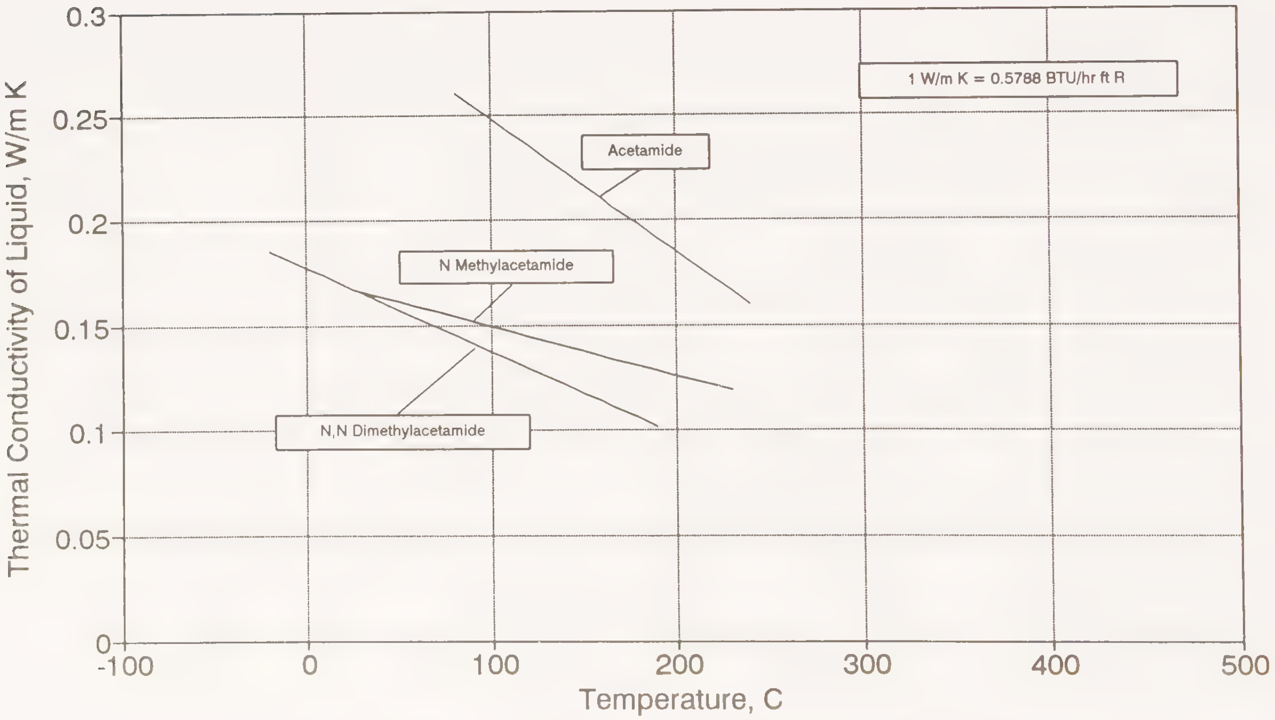

Figure 21-10 Thermal Conductivity of Liquid

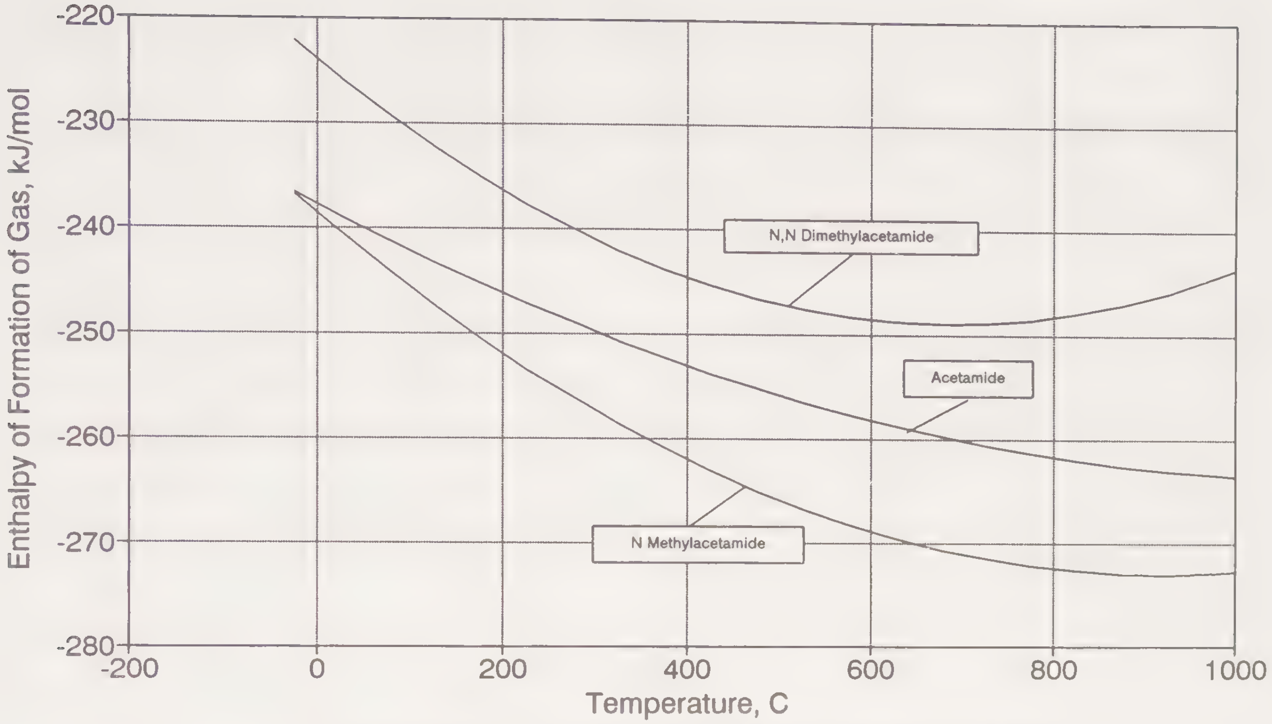

Figure 21-11 Enthalpy of Formation of Gas

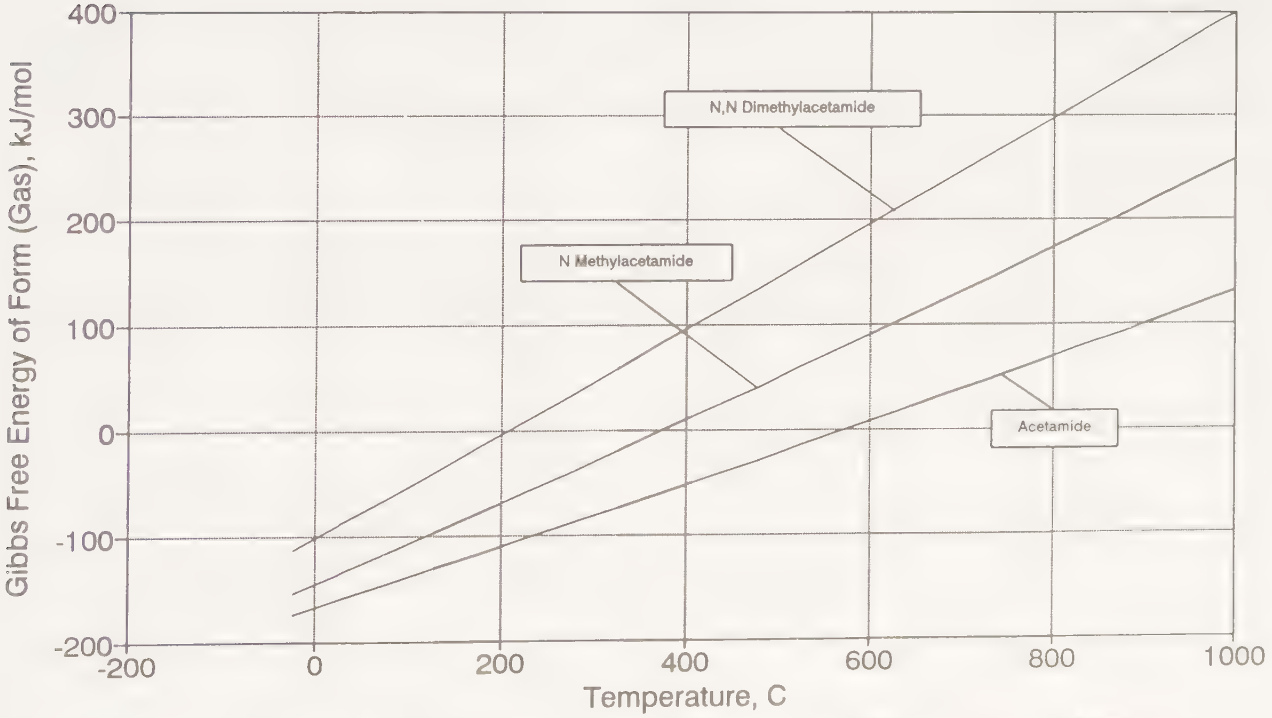

Figure 21-12 Gibbs Free Energy of Formation of Gas

Chapter 22

MISCELLANEOUS NITRILES

Robert W. Gallant and Carl L. Yaws

PHYSICAL PROPERTIES - Table 22-1

Property data from the literature (5,21,25,26,35,36,38,62,77,79,82,93,116-124) are given in Table 22-1. The critical constants were selected from the DIPPR project (5). Additional property data such as acentric factor, enthalpy of formation and explosion limits in air are also available.

VAPOR PRESSURE - Figure 22-1

Results from the DIPPR project (5) were selected for vapor pressure from very low temperatures to the critical point. Correlation of data for vapor pressure as a function of temperature was accomplished using Equation (1-1). Results from this equation (Antoine-type with extended terms) are in favorable agreement with experimental data. Errors are about 5% or less in most cases.

HEAT OF VAPORIZATION - Figure 22-2

Results from the DIPPR project (5) were selected for heat of vaporization for temperatures ranging from melting point to critical point. Equation (1-2) was used for correlation of the data as a function of temperature. Reliability of results is fair with possible errors of 10%.

LIQUID DENSITY - Figure 22-3

Results from the DIPPR project (5) were selected for liquid density from low temperatures at the melting point to higher temperatures up to the critical point. Equation (1-3) was used for correlation of the data as a function of temperature. Results from the correlation are in favorable agreement with data. Deviations are less than 3% in most cases.

SURFACE TENSION - Figure 22-4

Results from the DIPPR project (5) were selected for surface tension for temperatures from melting point to critical point. Using data from the literature, correlation for surface tension as a function of temperature over the full liquid range was achieved by Equation (1-4). Accuracy is favorable with errors being about 3% or less in most cases.

HEAT CAPACITY - Figures 22-5 and 22-6

Results from the DIPPR project (5) were selected for heat capacity of ideal gas. Correlation of data was

accomplished using Equation (1-5a). Results are in favorable agreement with data. Errors are about 5% or less in most cases.

Results from the DIPPR project (5) were selected for heat capacity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data were correlated with a series expansion in temperature, Equation (1-6). Results are in fair agreement with data. Errors are about 10% or less in most cases.

VISCOSITY - Figures 22-7 and 22-8

Results from the DIPPR project (5) were selected for viscosity of gas. Data for gas viscosity as a function of temperature were correlated using Equation (1-7). Results are in fair agreement with data. Errors are about 10% or less in most cases.

Results from the DIPPR project (5) were selected for viscosity of liquid. Temperatures from below the boiling point to temperatures above the boiling point are covered for most of the compounds. Data for liquid viscosity as a function of temperature were correlated using the de Guzman - Andrade equation with extended terms, Equation (1-8). Correlation results and data are in fair agreement with errors being about 10% or less in most cases.

THERMAL CONDUCTIVITY - Figures 22-9 and 22-10

Results from the DIPPR project (5) were selected for thermal conductivity of gas. Data for gas thermal conductivity as a function of temperature were correlated using Equation (1-9). Reliability of results is fair with errors less then 10% in most cases.

Results from the DIPPR project (5) were selected for thermal conductivity of liquid. The coverage applies to temperatures from below the boiling point to temperatures above the boiling point for most of the compounds. Data for liquid thermal conductivity as a function of temperature were correlated using a series expansion in temperature, Equation (1-10). Reliability of results is fair with possible errors of 10% in most cases.

ENTHALPY OF FORMATION - Figure 22-11

The data compilation of DIPPR project (5) was selected for enthalpy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for enthalpy of formation of the ideal gas is a series expansion in temperature, Equation (1-11). Results from the correlation are in favorable agreement with data.

GIBB'S FREE ENERGY OF FORMATION - Figure 22-12

The data compilation of DIPPR project (5) was selected for Gibb's free energy of formation of ideal gas. The values at 25 C were extended to higher temperatures by integration of the appropriate equations (76) which involve gas heat capacities. Data for Gibb's free energy of formation of the ideal gas is a series expansion in temperature, Equation (1-12). Results from the correlation are in favorable agreement with data.

Table 22-1 Physical Properties

1. Name	Acrylonitrile	Adiponitrile
2. Formula	C3H3N	C6H8N2
3. Molecular Weight, g/mol	53.064	108.143
4. Critical Temperature, K	535.00	781.00
5. Critical Pressure, bar	44.8	28.3
6. Critical Volume, ml/mol	212.0	406.0
7. Critical Compressibility Factor	0.214	0.177
8. Acentric Factor	0.3498	0.6723
9. Melting Point, K	189.63	275.64
10. Boiling Point @ 1 atm, K	350.50	568.15
11. Heat of Vaporization @ BP, kJ/kg	585.34	532.06
12. Density of Liquid @ 25 C, g/ml	0.801	0.960
13. Surface Tension @ 25 C, dynes/cm	15.93	45.84
14. Heat Capacity of Gas @ 25 C, J/g K	1.214	1.297
15. Heat Capacity of Liquid @ 25 C, J/g K	2.05	1.19
16. Viscosity of Gas @ 25 C, micropoise	65.49	61.55
17. Viscosity of Liquid @ 25 C, centipoise	0.335	5.661
18. Thermal Conductivity of Gas @ 25 C, W/m K	0.009	0.005
19. Thermal Conductivity of Liquid @ 25 C, W/m K	0.169	0.174
20. Enthalpy of Formation of Gas @ 25 C, kJ/mol	183.62	149.07
21. Gibbs Free Energy of Formation of Gas @ 25 C, kJ/mol	193.44	252.53
22. Flash Point, K	273.15	366.15
23. Autoignition Temperature, K	754.26	823.15
24. Lower Explosion Limit in Air, vol %	2.4	1.7
25. Upper Explosion Limit in Air, vol %	17.3	5.0
26. Solubility in Water @ 25 C, ppm(wt)	73500 @ 20 C	------

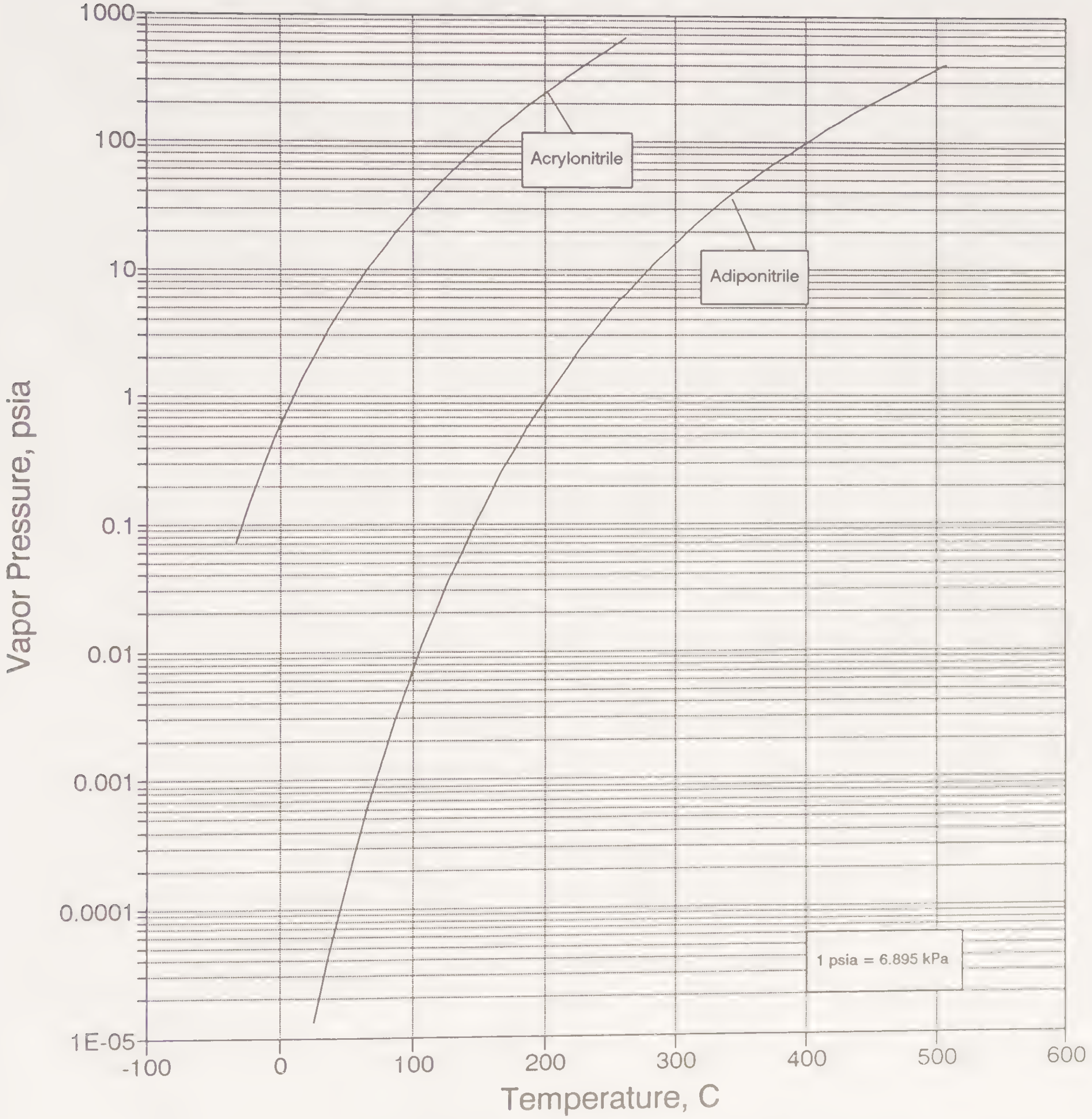

Figure 22-1 Vapor Pressure

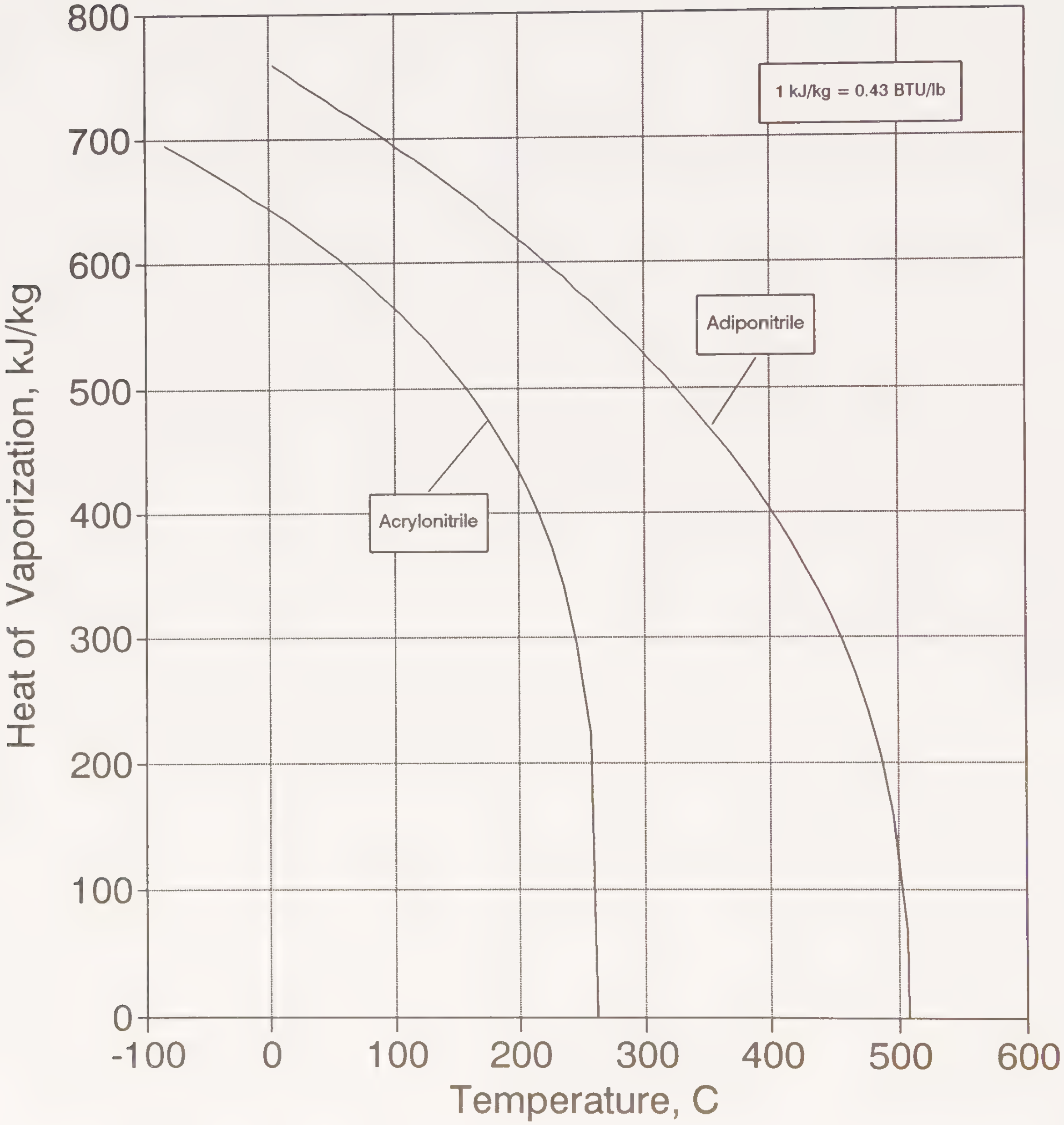

Figure 22-2 Heat of Vaporization

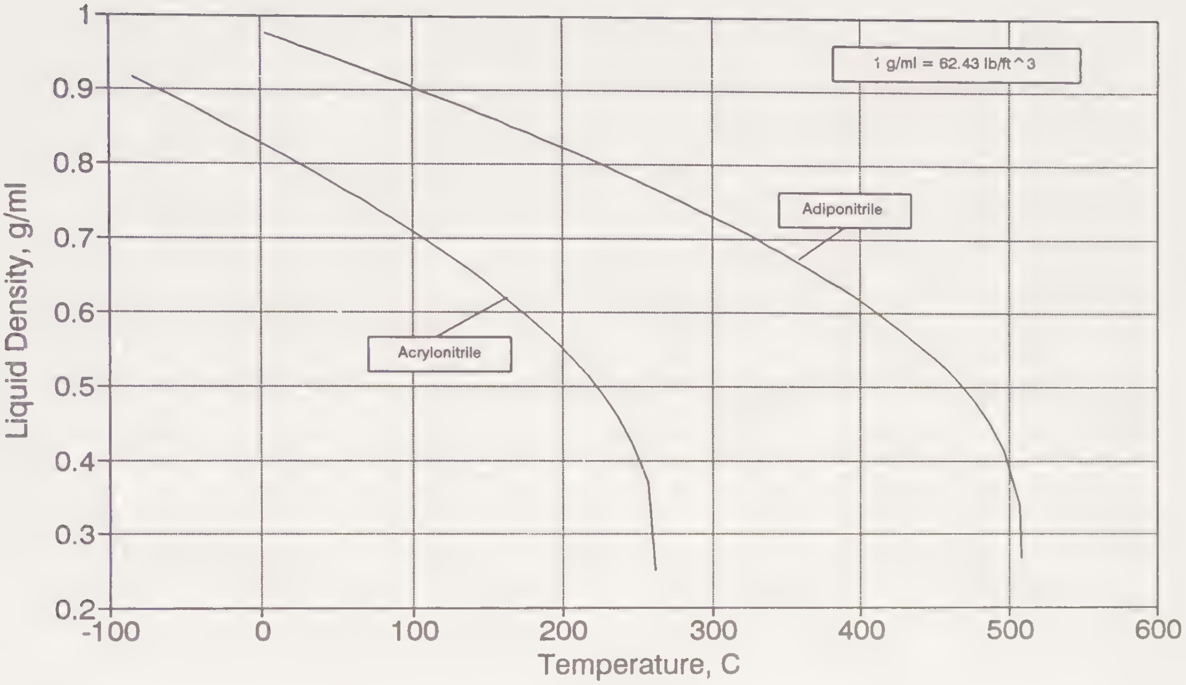

Figure 22-3 Liquid Density

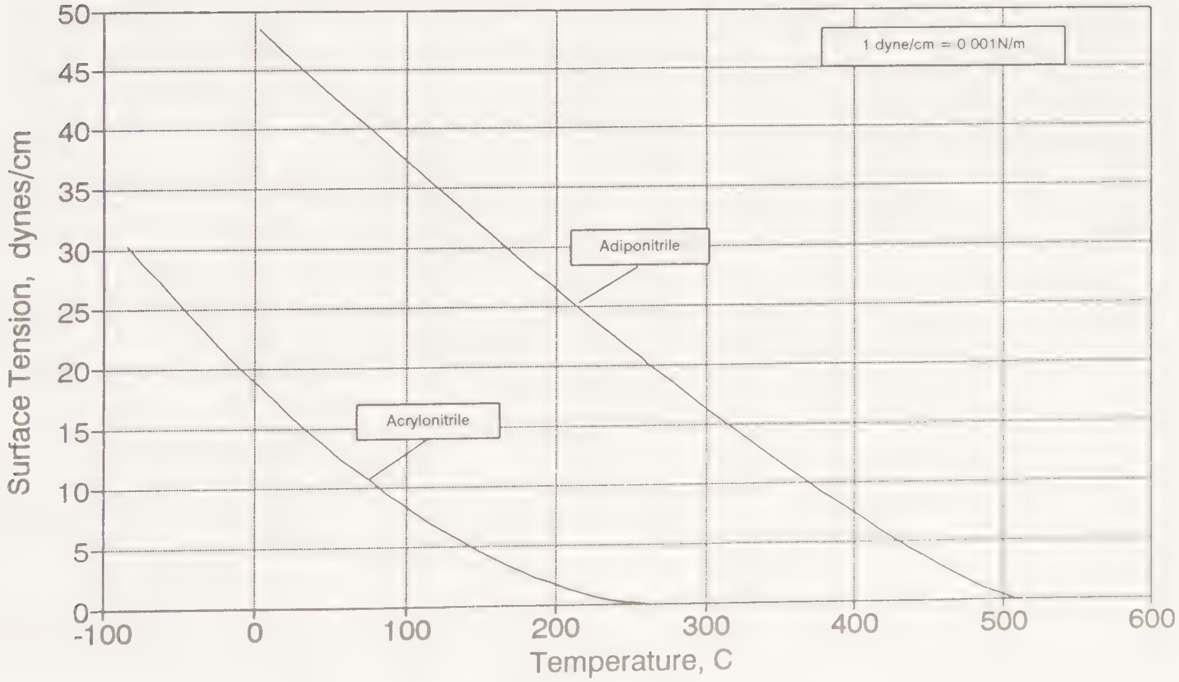

Figure 22-4 Surface Tension

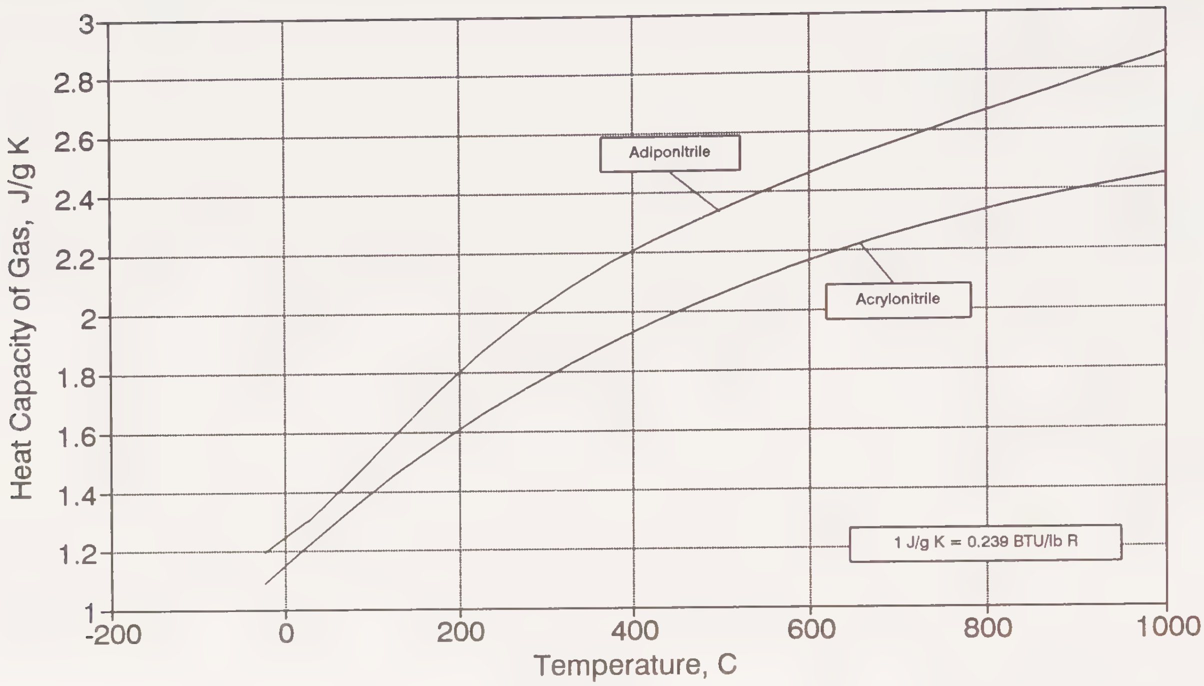

Figure 22-5 Heat Capacity of Gas

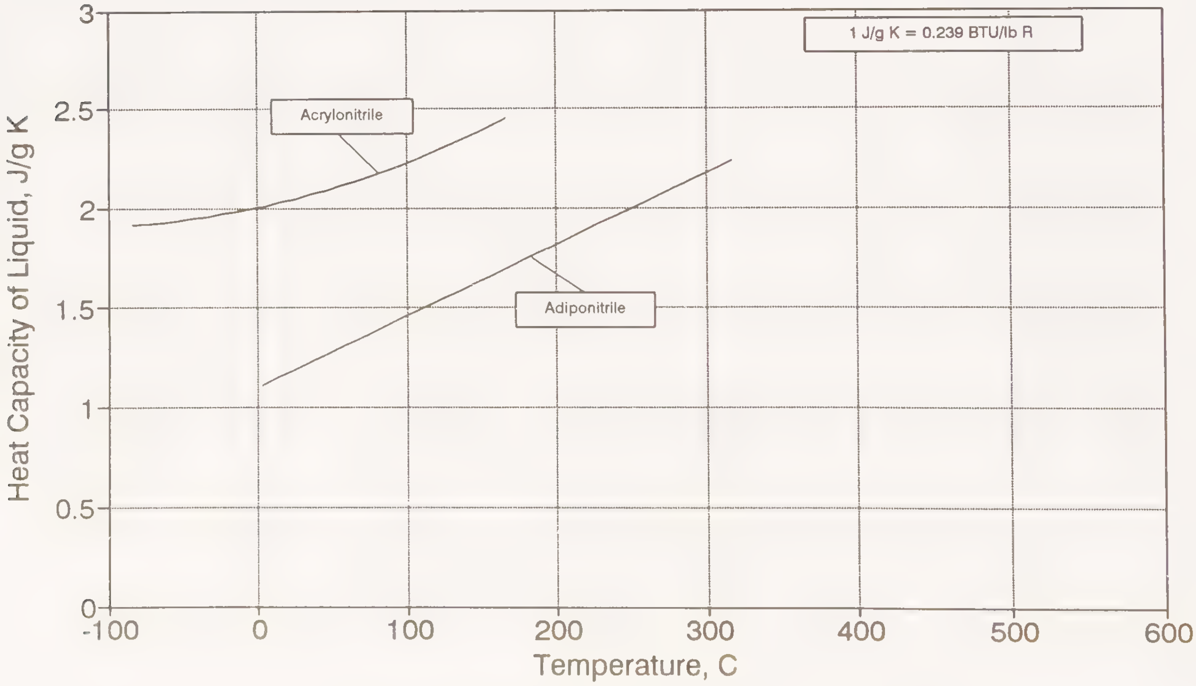

Figure 22-6 Heat Capacity of Liquid

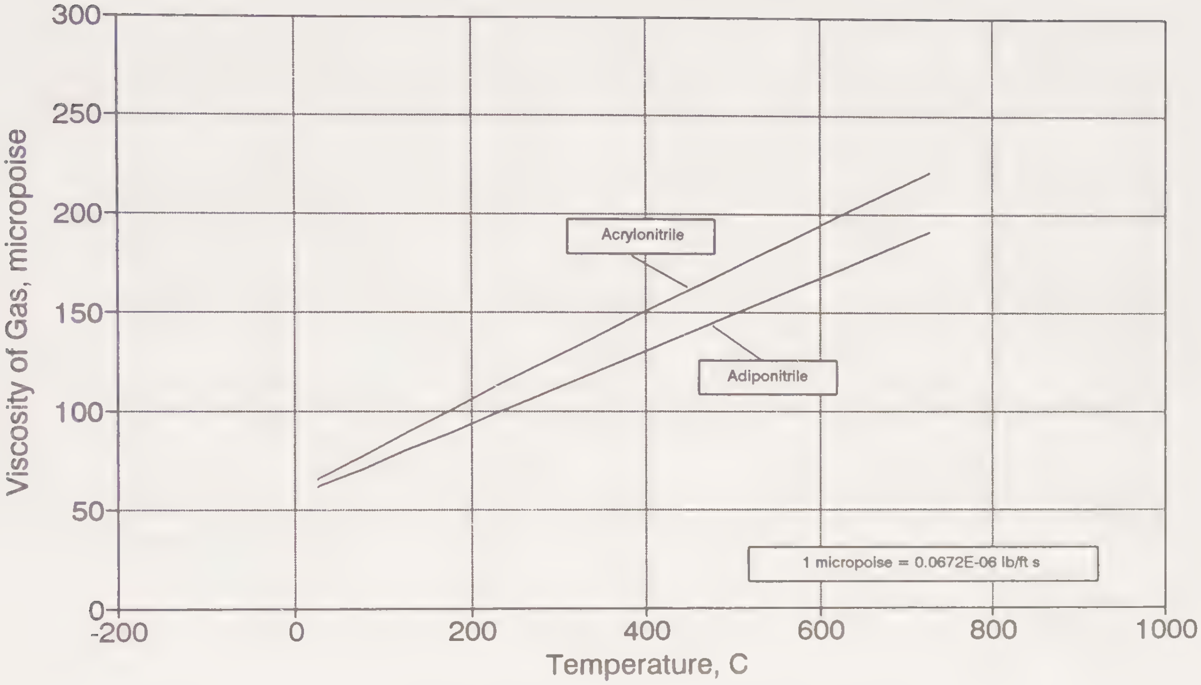

Figure 22-7 Viscosity of Gas

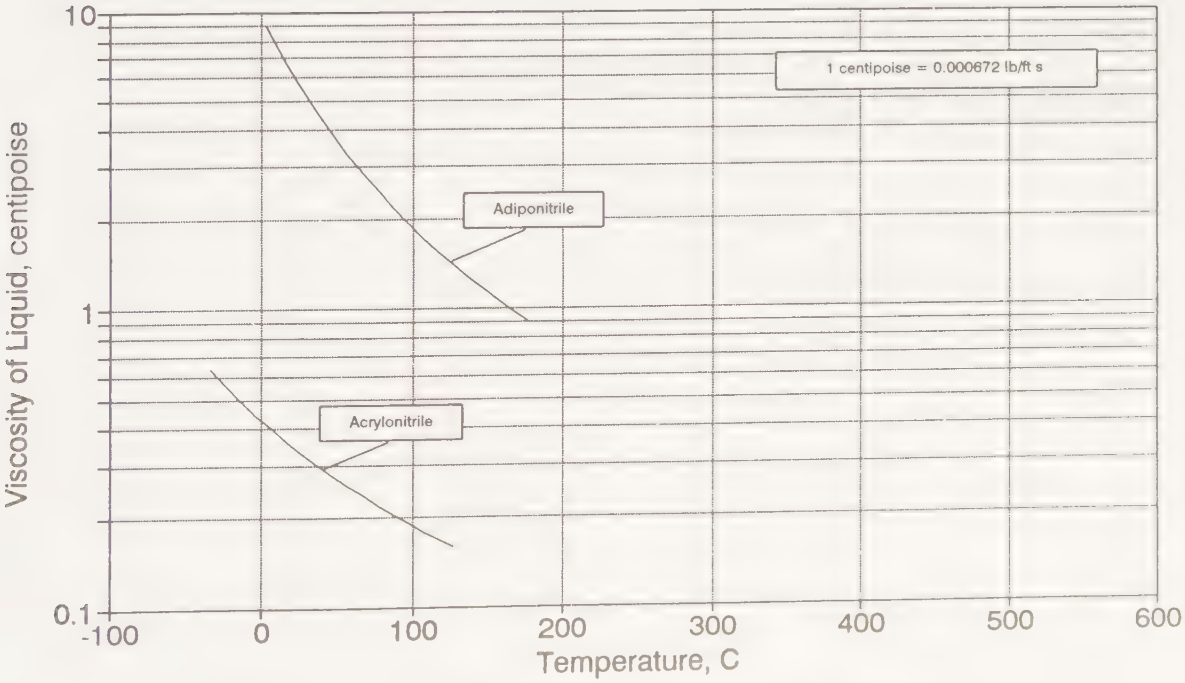

Figure 22-8 Viscosity of Liquid

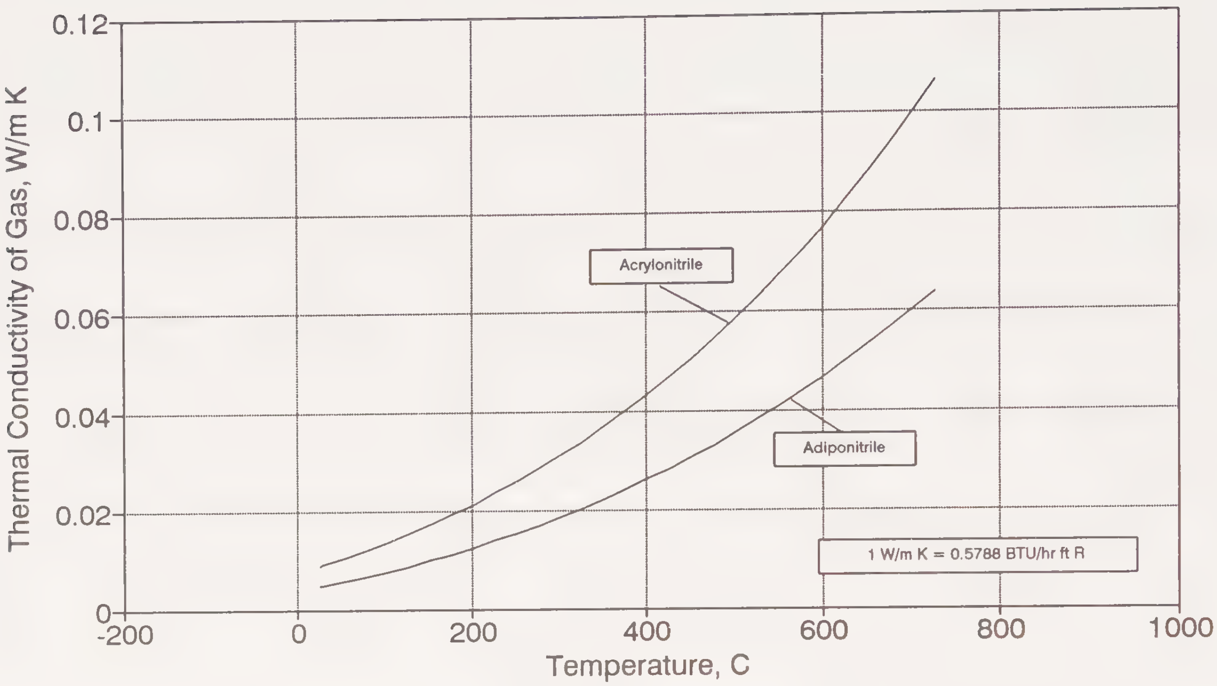

Figure 22-9 Thermal Conductivity of Gas

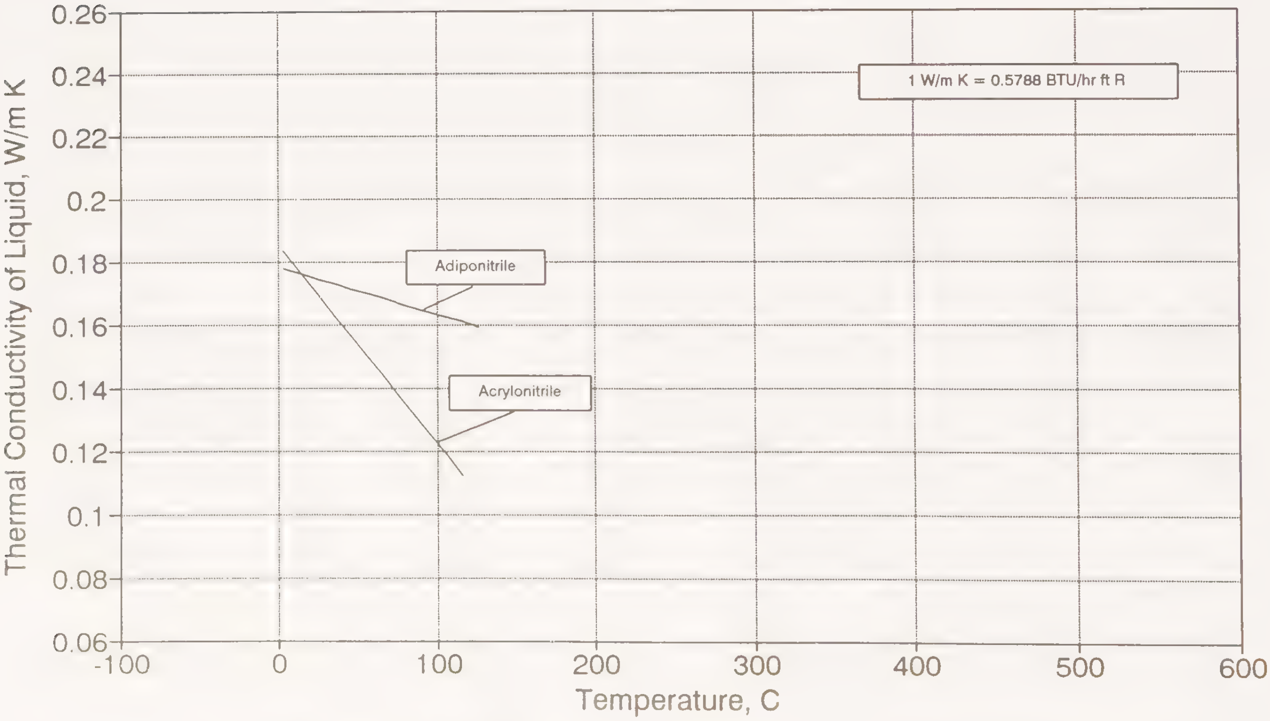

Figure 22-10 Thermal Conductivity of Liquid

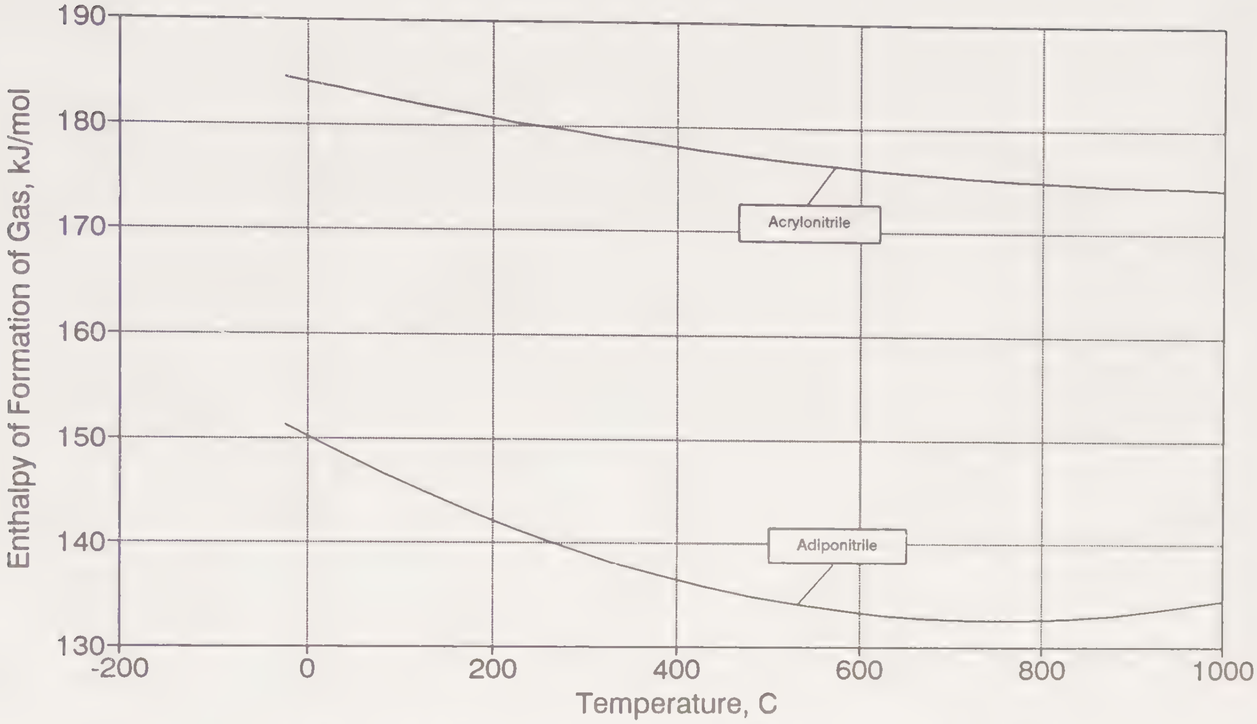

Figure 22-11 Enthalpy of Formation of Gas

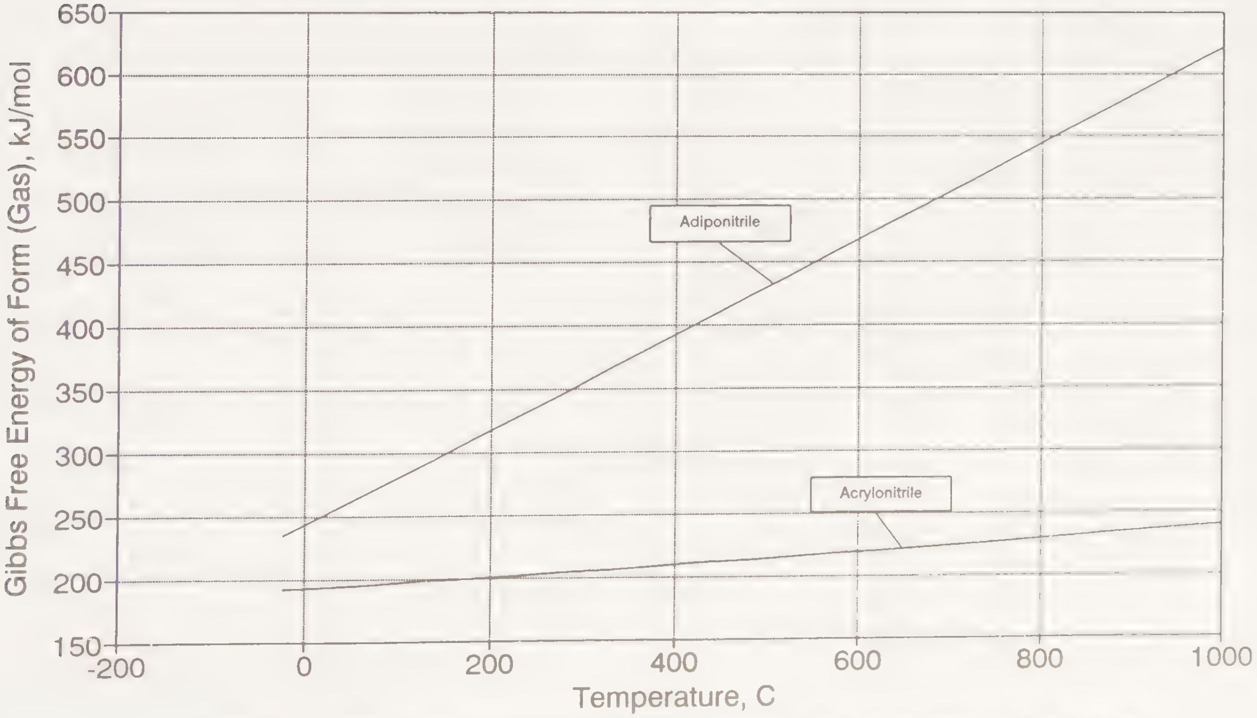

Figure 22-12 Gibbs Free Energy of Formation of Gas

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Appendix A

CONVERSION TABLES

1. **Temperature**
   To convert from Centigrade to:
      Kelvin, add 273.15
      Rankine, multiply Kelvin by 1.8
      Fahrenheit, multiply Centigrade by 1.8 and add 32

2. **Pressure**
   To convert from psia to:
      kPa, multiply by 6.895
      psig, subtract 14.7
      mm Hg, multiply by 51.7
      atmospheres, divide by 14.7
      bars, divide by 14.89

3. **Heat of Vaporization**
   To convert from kJ/kg to:
      BTU/lb, multiply by 0.43
      cal/gram, multiply by 0.239

4. **Density**
   To convert from g/ml to:
      lb/ft^3, multiply by 62.43
      lb/gallon, multiply by 8.345

5. **Surface Tension**
   To convert from dynes/cm to:
      N/m, multiply by 0.001

6. **Heat Capacity**
   To convert from J/g K to:
      BTU/lb R, multiply by 0.239
      cal/gram K, multiply by 0.239

7. **Viscosity**
   To convert from micropoise to:
      lb/ft s, multiply by 0.0672E-06
      centipoise, multiply by 1.0E-04
      poise, multiply by 1.0E-06
      Pa s (pascal seconds), multiply by 1.0E-07

   To convert from centipoise to:
      lb/ft s, multiply by 0.000672
      micropoise, multiply by 10,000
      poise, multiply by 0.01
      Pa s (pascal seconds), multiply by 0.001

8. **Thermal Conductivity**
   To convert from W/m K to:
      BTU/hr ft R, multiply by 0.5788
      calorie/cm s K, multiply by 0.002388

9. **Enthalpy of Formation**
   To convert from kJ/mol to:
      kcal/mol, multiply by 0.239

10. **Gibb's Free Energy of Formation**
   To convert from kJ/mol to:
      kcal/mol, multiply by 0.239

Appendix B

COMPOUND INDEX BY FORMULA

Formula	Name	Synonym	Page
Ar	argon		61(Vol 3)
Br2	bromine		110(Vol 3)
CBrF3	bromotrifluoromethane		235(Vol 1)
CClF3	chlorotrifluoromethane	fluorocarbon-13	205(Vol 1)
CCl2F2	dichlorodifluoromethane	fluorocarbon-12	205(Vol 1)
CCl2O	phosgene		16(Vol 2)
CCl3F	trichlorofluoromethane	fluorocarbon-11	205(Vol 1)
CCl4	carbon tetrachloride		44(Vol 1)
CF4	tetrafluoromethane	fluorocarbon-14	205(Vol 1)
CO	carbon monoxide		1(Vol 3)
COS	carbonyl sulfide		90(Vol 3)
CO2	carbon dioxide		1(Vol 3)
CS2	carbon disulfide		206(Vol 2)
CHClF2	chlorodifluoromethane	fluorocarbon-21	215(Vol 1)
CHCl2F	dichlorofluoromethane	fluorocarbon-22	215(Vol 1)
CHCl3	chloroform	trichloromethane	44(Vol 1)
CHF3	trifluoromethane	fluorocarbon-23	225(Vol 1)
CHN	hydrogen cyanide		126(Vol 2)
CH2Cl2	methylene chloride	dichloromethane	44(Vol 1)
CH2O	formaldehyde		6(Vol 2)
CH2O2	formic acid		26(Vol 2)
CH3Br	methyl bromide		235(Vol 1)
CH3Cl	methyl chloride		44(Vol 1)
CH3NO	formamide		194(Vol 4)
CH3NO2	nitromethane		136(Vol 2)
CH4	methane		1(Vol 1)
CH4O	methanol		74(Vol 1)
CH4S	methanethiol		206(Vol 2)
CH5N	methylamine		96(Vol 2)
C2Cl2F4	1,2-dichloro-1,1,2,2-tertafluoroethane	fluorocarbon-114	215(Vol 1)
C2Cl3F3	1,1,2-trichloro-1,2,2-trifluoroethane	fluorocarbon-113	215(Vol 1)
C2Cl4	perchloroethylene		54(Vol 1)
C2F6	hexafluoroethane	fluorocarbon-116	225(Vol 1)
C2HCl3	trichloroethylene		54(Vol 1)
C2HCl3O	chloral		16(Vol 2)
C2H2	acetylene	ethyne	24(Vol 1)
C2H2Cl2	vinylidene chloride		54(Vol 1)
C2H2Cl2	cis-1,2-dichloroethylene		195(Vol 1)
C2H2Cl2	trans-1,2-dichloroethylene		195(Vol 1)
C2H2Cl4	1,1,2,2-tertachloroethane		195(Vol 1)

C2H2F2 vinylidene fluoride..............................225(Vol 1)
C2H3Cl vinyl chloride..............................54(Vol 1)
C2H3ClO acetyl chloride..............................16(Vol 2)
C2H3Cl3 methyl chloroform........1,1,1-trichloroethane..195(Vol 1)
C2H3F vinyl fluoride..............................225(Vol 1)
C2H3N acetonitrile..............................126(Vol 2)
C2H4 ethylene...............ethene..................14(Vol 1)
C2H4Br2 ethylene dibromide......1,2-dibromoethane.....235(Vol 1)
C2H4Cl2 ethylene dichloride.....1,2-dichloroethane.....64(Vol 1)
C2H4O ethylene oxide..............................104(Vol 1)
C2H4O acetaldehyde..............................6(Vol 2)
C2H4O2 acetic acid..............................26(Vol 2)
C2H4O2 methyl formate..............................114(Vol 4)
C2H5Br ethyl bromide...........bromoethane............235(Vol 1)
C2H5Cl ethyl chloride..........chloroethane...........64(Vol 1)
C2H5NO acetamide..............................204(Vol 4)
C2H5NO n methylformamide..............................194(Vol 4)
C2H5NO2 nitroethane..............................136(Vol 2)
C2H6 ethane..............................1(Vol 1)
C2H6O ethanol................ethyl alcohol..........74(Vol 1)
C2H6O methyl ether..............................46(Vol 2)
C2H6O2 ethylene glycol..............................114(Vol 1)
C2H6S ethanethiol..............................206(Vol 2)
C2H6S dimethyl sulfide..............................206(Vol 2)
C2H7N dimethylamine..............................96(Vol 2)
C2H7N ethylamine..............................106(Vol 2)
C2H8N ethylenediamine..............................184(Vol 4)
C3H3N acrylonitrile..............................214(Vol 4)
C3H4 methyl acetylene........propyne................24(Vol 1)
C3H4 propadiene..............allene.................34(Vol 1)
C3H4O acrolein..............................16(Vol 2)
C3H4O2 acrylic acid..............................76(Vol 2)
C3H5ClO epichlorohydrin..............................104(Vol 1)
C3H5N propionitrile..............................126(Vol 2)
C3H6 propylene..............propene................14(Vol 1)
C3H6 cyclopropane..............................176(Vol 2)
C3H6Cl2 propylene dichloride....1,2-dichloropropane....64(Vol 1)
C3H6O propylene oxide..............................104(Vol 1)
C3H6O allyl alcohol..............................94(Vol 1)
C3H6O prionaldehyde..............................6(Vol 2)
C3H6O acetone..............................36(Vol 2)
C3H6O2 ethyl formate..............................114(Vol 4)
C3H6O2 propionic acid..............................26(Vol 2)
C3H6O2 methyl acetate..............................66(Vol 2)
C3H7Cl propyl chloride.........1-chloropropane........64(Vol 1)
C3H7NO n,n dimethylformamide..............................194(Vol 4)
C3H7NO n methylacetamide..............................204(Vol 4)
C3H7NO2 1-nitropropane..............................136(Vol 2)
C3H7NO2 2-nitropropane..............................136(Vol 2)

C3H8	propane		1(Vol 1)
C3H8O	propanol	propyl alcohol	74(Vol 1)
C3H8O	isopropanol	isopropyl alcohol	84(Vol 1)
C3H8O2	propylene glycol	1,2-propylene glycol	135(Vol 1)
C3H8O3	glycerine	glycerol	135(Vol 1)
C3H9N	propylamine		174(Vol 4)
C3H9N	trimethylamine		96(Vol 2)
C3H9N	isopropylamine		116(Vol 2)
C4H4O	furan		56(Vol 2)
C4H4O2	furfural		56(Vol 2)
C4H6	1-butyne		24(Vol 1)
C4H6	2-butyne		24(Vol 1)
C4H6	1,2-butadiene		34(Vol 1)
C4H6	1,3-butadiene		34(Vol 1)
C4H6O2	vinyl acetate		66(Vol 2)
C4H6O2	methyl acrylate		76(Vol 2)
C4H6O3	acetic anhydride		86(Vol 2)
C4H6O4	succinic acid		54(Vol 4)
C4H7N	butyronitrile		126(Vol 2)
C4H8	1-butene		14(Vol 1)
C4H8	trans 2-butene		14(Vol 1)
C4H8	cis 2-butene		14(Vol 1)
C4H8	isobutylene	2-methylpropene	175(Vol 1)
C4H8	cyclobutane		176(Vol 2)
C4H8O	butylene oxide	1,2-butylene oxide	104(Vol 1)
C4H8O	butyraldehyde		6(Vol 2)
C4H8O	methyl ethyl ketone		36(Vol 2)
C4H8O	tetrahydrofuran		56(Vol 2)
C4H8O2	butyric acid		26(Vol 2)
C4H8O2	dioxane		56(Vol 2)
C4H8O2	ethyl acetate		66(Vol 2)
C4H8O2	propyl formate		114(Vol 4)
C4H9NO	n,n dimethylacetamide		204(Vol 4)
C4H10	butane		1(Vol 1)
C4H10	isobutane	2-methylpropane	175(Vol 1)
C4H10O	butanol	butyl alcohol	74(Vol 1)
C4H10O	isobutyl alcohol		84(Vol 1)
C4H10O	sec-butyl alcohol		84(Vol 1)
C4H10O	tert-butyl alcohol		84(Vol 1)
C4H10O	ethyl ether		46(Vol 2)
C4H10O2	1,3 butylene glycol(1,3 butanediol)		154(Vol 4)
C4H10O2	1,4 butylene glycol(1,4 butanediol)		154(Vol 4)
C4H10O2	2,3 butylene glycol(2,3 butanediol)		154(Vol 4)
C4H10O3	diethylene glycol		114(Vol 1)
C4H11N	diethylamine		106(Vol 2)
C4H11N	butylamine		116(Vol 2)
C5H5N	pyridine		146(Vol 2)
C5H8	isoprene	2-methyl-1,3-butadiene	175(Vol 1)
C5H8	cyclopentene		186(Vol 2)

C5H8O2 ethyl acrylate........76(Vol 2)
C5H8O2 methyl methacrylate........76(Vol 2)
C5H10 1-pentene........isopentene........165(Vol 1)
C5H10 cyclopentane........176(Vol 2)
C5H10O diethyl ketone........84(Vol 4)
C5H10O methyl isopropyl ketone........84(Vol 4)
C5H10O methyl propyl ketone........84(Vol 4)
C5H10O pentanal........1(Vol 4)
C5H10O2 butyl formate........124(Vol 4)
C5H10O2 isobutyl formate........124(Vol 4)
C5H10O2 isopropyl acetate........134(Vol 4)
C5H10O2 pentanoic acid........24(Vol 4)
C5H10O2 propyl acetate........134(Vol 4)
C5H12 pentane........155(Vol 1)
C5H12 isopentane........2-methylbutane........175(Vol 1)
C5H12O ethyl propyl ether........104(Vol 4)
C5H12O methyl sec-butyl ether........104(Vol 4)
C5H12O methyl tert-butyl ether........104(Vol 4)
C5H12O 1-pentanol........1-amyl alcohol........94(Vol 1)
C6H5Br bromobenzene........196(Vol 2)
C6H5Cl chlorobenzene........196(Vol 2)
C6H5F fluorobenzene........196(Vol 2)
C6H6 benzene........156(Vol 2)
C6H7N aniline........146(Vol 2)
C6H8N2 adiponitrile........214(Vol 4)
C6H10 cyclohexene........186(Vol 2)
C6H10O3 propionic anhydride........86(Vol 2)
C6H10O4 adipic acid........54(Vol 4)
C6H12 1-hexene........165(Vol 1)
C6H12 cyclohexane........176(Vol 2)
C6H12 methyl cyclopentane........159(Vol 3)
C6H12O ethyl isopropyl ketone........94(Vol 4)
C6H12O ethyl propyl ketone........94(Vol 4)
C6H12O hexanal........1(Vol 4)
C6H12O methyl butyl ketone........94(Vol 4)
C6H12O methyl isobutyl ketone........94(Vol 4)
C6H12O2 butyl acetate........144(Vol 4)
C6H12O2 hexanoic acid........24(Vol 4)
C6H12O2 sec-butyl acetate........144(Vol 4)
C6H12O2 tert-butyl acetate........144(Vol 4)
C6H14 hexane........155(Vol 1)
C6H14 2-methylpentane........isohexane........185(Vol 1)
C6H14O 1-hexanol........1-hexyl alcohol........94(Vol 1)
C6H14O propyl ether........46(Vol 2)
C6H14O2 hexamethylene glycol(1,6 hexanediol)........164(Vol 4)
C6H14O2 hexylene glycol(2 methyl 2,4 pentanediol)........164(Vol 4)
C6H14O3 dipropylene glycol........135(Vol 1)
C6H14O4 triethylene gylcol........114(Vol 1)
C6H15N diisopropylamine........116(Vol 2)

C6H15N	dipropylamine		174(Vol 4)
C6H15N	triethylamine		106(Vol 2)
C6H16N2	hexamethylenediamine		184(Vol 4)
C7H7Cl	benzyl chloride		196(Vol 2)
C7H8	toluene		166(Vol 2)
C7H14	1-heptene		165(Vol 1)
C7H14	ethyl cyclopentane		159(Vol 3)
C7H14	methyl cyclohexane		169(Vol 3)
C7H14O	heptanal		1(Vol 4)
C7H14O2	heptanoic acid		24(Vol 4)
C7H16	heptane		155(Vol 1)
C7H16	2-methylhexane		185(Vol 1)
C7H16O	1-heptanol	1-heptyl alcohol	94(Vol 1)
C8H8	styrene		186(Vol 2)
C8H10	ethylbenzene		156(Vol 2)
C8H10	m-xylene		166(Vol 2)
C8H10	o-xylene		166(Vol 2)
C8H10	p-xylene		166(Vol 2)
C8H12	cyclooctadiene		186(Vol 2)
C8H14O3	butyric anhydride		86(Vol 2)
C8H16	1-octene		165(Vol 1)
C8H16	propyl cyclopentane		159(Vol 3)
C8H16	ethyl cyclohexane		169(Vol 3)
C8H16O	octanal		14(Vol 4)
C8H16O2	octanoic acid		34(Vol 4)
C8H18	octane		155(Vol 1)
C8H18	isooctane	2,2,4-trimethylpentane	185(Vol 1)
C8H18	2-methylheptane		185(Vol 1)
C8H18O	butyl ether		46(Vol 2)
C8H18O	octanol		64(Vol 4)
C8H19N	dibutylamine		116(Vol 2)
C9H12	propylbenzene		156(Vol 2)
C9H12	cumene		156(Vol 2)
C9H18	propyl cyclohexane		169(Vol 3)
C9H21N	tripropylamine		174(Vol 4)
C10H8	naphthelene		209(Vol 3)
C10H14	butyl benzene		179(Vol 3)
C10H18	cis-decahydronaphthelene		209(Vol 3)
C10H18	trans-decahydronaphthelene		209(Vol 3)
C10H20	decene		139(Vol 3)
C10H20O	decanal		14(Vol 4)
C10H20O2	decanoic acid		34(Vol 4)
C10H22	decane		119(Vol 3)
C10H22O	decanol		64(Vol 4)
C11H16	pentyl benzene		179(Vol 3)
C12H18	hexyl benzene		179(Vol 3)
C12H24	dodecene		139(Vol 3)
C12H24O	dodecanal		14(Vol 4)
C12H24O2	dodecanoic acid		34(Vol 4)

C12H26 dodecane.....119(Vol 3)
C12H26O dodecanol.....64(Vol 4)
C13H20 heptyl benzene.....189(Vol 3)
C14H22 octyl benzene.....189(Vol 3)
C14H28 tetradecene.....139(Vol 3)
C14H28O2 tetradecanoic acid.....44(Vol 4)
C14H30 tetradecane.....119(Vol 3)
C14H30O tetradecanol.....74(Vol 4)
C15H24 nonyl benzene.....189(Vol 3)
C16H26 decyl benzene.....199(Vol 3)
C16H32 hexadecene.....149(Vol 3)
C16H32O2 hexadecanoic acid.....44(Vol 4)
C16H34 hexadecane.....129(Vol 3)
C16H34O hexadecanol.....74(Vol 4)
C17H28 undecyl benzene.....199(Vol 3)
C18H30 dodecyl benzene.....199(Vol 3)
C18H36 octadecene.....149(Vol 3)
C18H36O2 octadecanoic acid.....44(Vol 4)
C18H38 octadecane.....129(Vol 3)
C18H38O octadecanol.....74(Vol 4)
C20H40 eicosene.....149(Vol 3)
C20H42 eicosane.....129(Vol 3)
Cl2 chlorine.....110(Vol 3)
F2 fluorine.....110(Vol 3)
HBr hydrogen bromide.....100(Vol 3)
HCl hydrogen chloride.....100(Vol 3)
HF hydrogen fluoride.....100(Vol 3)
HI hydrogen iodide.....100(Vol 3)
H2 hydrogen.....52(Vol 3)
H2O water.....216(Vol 2)
H2S hydrogen sulfide.....90(Vol 3)
He helium.....52(Vol 3)
I2 iodine.....110(Vol 3)
NH3 ammonia.....42(Vol 3)
NO nitric oxide.....70(Vol 3)
NO2 nitrogen dioxide.....70(Vol 3)
N2 nitrogen.....14(Vol 3)
N2O nitrous oxide.....70(Vol 3)
Ne neon.....61(Vol 3)
O2 oxygen.....14(Vol 3)
O3 ozone.....32(Vol 3)
SO2 sulfur dioxide.....80(Vol 3)
SO3 sulfur trioxide.....80(Vol 3)

Appendix C

COMPOUND INDEX BY NAME

Name	Synonym	Page
acetaldehyde		6(Vol 2)
acetamide		204(Vol 4)
acetic acid		26(Vol 2)
acetic anhydride		86(Vol 2)
acetone		36(Vol 2)
acetonitrile		126(Vol 2)
acetyl chloride		16(Vol 2)
acetylene	ethyne	24(Vol 1)
acrolein		16(Vol 2)
acrylic acid		76(Vol 2)
acrylonitrile		214(Vol 4)
adipic acid		54(Vol 4)
adiponitrile		214(Vol 4)
allyl alcohol		94(Vol 1)
ammonia		42(Vol 3)
aniline		146(Vol 2)
argon		61(Vol 3)
benzene		156(Vol 2)
benzyl chloride		196(Vol 2)
bromine		110(Vol 3)
bromobenzene		196(Vol 2)
bromotrifluoromethane		235(Vol 1)
1,2-butadiene		34(Vol 1)
1,3-butadiene		34(Vol 1)
butane		1(Vol 1)
butanol	butyl alcohol	74(Vol 1)
1-butene		14(Vol 1)
trans 2-butene		14(Vol 1)
cis 2-butene		14(Vol 1)
sec-butyl alcohol		84(Vol 1)
tert-butyl alcohol		84(Vol 1)
butylene oxide	1,2-butylene oxide	104(Vol 1)
butyl acetate		144(Vol 4)
sec-butyl acetate		144(Vol 4)
tert-butyl acetate		144(Vol 4)
butyl amine		116(Vol 2)
butyl benzene		179(Vol 3)
butyl ether		46(Vol 2)
butyl formate		124(Vol 4)
2,3 butylene glycol(2,3 butanediol)		154(Vol 4)

1,3 butylene glycol(1,3 butanediol)...........154(Vol 4)
1,4 butylene glycol(1,4 butanediol)...........154(Vol 4)
1-butyne...................................24(Vol 1)
2-butyne...................................24(Vol 1)
butyraldehyde...............................6(Vol 2)
butyric acid...............................26(Vol 2)
butyric anhydride..........................86(Vol 2)
butyronitrile.............................126(Vol 2)
carbon dioxide..............................1(Vol 3)
carbon disulfide..........................206(Vol 2)
carbon monoxide.............................1(Vol 3)
carbon tetrachloride.......................44(Vol 1)
carbonyl sulfide...........................90(Vol 3)
chloral....................................16(Vol 2)
chlorine..................................110(Vol 3)
chlorobenzene.............................196(Vol 2)
chlorodifluoromethane...fluorocarbon-21.......215(Vol 1)
chloroform.............trichloromethane......44(Vol 1)
chlorotrifluoromethane...fluorocarbon-13.......205(Vol 1)
cumene....................................156(Vol 2)
cyclobutane...............................176(Vol 2)
cyclohexane...............................176(Vol 2)
cyclohexene...............................186(Vol 2)
cyclooctadiene............................186(Vol 2)
cyclopentane..............................176(Vol 2)
cyclopentene..............................186(Vol 2)
cyclopropane..............................176(Vol 2)
cis-decahydronaphthelene..................209(Vol 3)
trans-decahydronaphthelene................209(Vol 3)
decanal....................................14(Vol 4)
decane....................................119(Vol 3)
decanoic acid..............................34(Vol 4)
decanol....................................64(Vol 4)
decene....................................139(Vol 3)
decyl benzene.............................199(Vol 3)
dibutylamine..............................116(Vol 2)
dichlorodifluoromethane..fluorocarbon-12.......205(Vol 1)
cis-1,2-dichloroethylene..................195(Vol 1)
trans-1,2-dichloroethylene................195(Vol 1)
dichlorofluoromethane....fluorocarbon-22.......215(Vol 1)
1,2-dichloro-1,1,
 2,2-tertafluoroethane...fluorocarbon-114......215(Vol 1)
diethyl ketone.............................84(Vol 4)
diethylamine..............................106(Vol 2)
diethylene glycol.........................114(Vol 1)
diisopropylamine..........................116(Vol 2)
dimethyl sulfide..........................206(Vol 2)
n,n dimethylacetamide.....................204(Vol 4)
dimethylamine..............................96(Vol 2)

n,n dimethylformamide............................194(Vol 4)
dioxane...56(Vol 2)
dipropylamine...................................174(Vol 4)
dipropylene glycol...............................135(Vol 1)
dodecanal.......................................14(Vol 4)
dodecane...119(Vol 3)
dodecanoic acid.................................34(Vol 4)
dodecanol.......................................64(Vol 4)
dodecene...139(Vol 3)
dodecyl benzene..................................199(Vol 3)
eicosane...129(Vol 3)
eicosene...149(Vol 3)
epichlorohydrin..................................104(Vol 1)
ethane...1(Vol 1)
ethanethiol......................................206(Vol 2)
ethanol.................ethyl alcohol.........74(Vol 1)
ethyl acetate....................................66(Vol 2)
ethyl acrylate...................................76(Vol 2)
ethyl amine......................................106(Vol 2)
ethyl benzene....................................156(Vol 2)
ethyl bromide...........bromoethane...........235(Vol 1)
ethyl chloride..........chloroethane..........64(Vol 1)
ethyl cyclohexane................................169(Vol 3)
ethyl cyclopentane...............................159(Vol 3)
ethyl ether......................................46(Vol 2)
ethyl formate...................................114(Vol 4)
ethyl isopropyl ketone..........................94(Vol 4)
ethyl propyl ether..............................104(Vol 4)
ethyl propyl ketone.............................94(Vol 4)
ethylene................ethene................14(Vol 1)
ethylene dibromide......1,2-dibromoethane......235(Vol 1)
ethylene dichloride.....1,2-dichloroethane.....64(Vol 1)
ethylene glycol..................................114(Vol 1)
ethylene oxide...................................104(Vol 1)
ethylenediamine.................................184(Vol 4)
fluorine...110(Vol 3)
fluorobenzene....................................196(Vol 2)
formaldehyde.....................................6(Vol 2)
formamide.......................................194(Vol 4)
formic acid......................................26(Vol 2)
furan..56(Vol 2)
furfural...56(Vol 2)
glycerine...............glycerol..............135(Vol 1)
helium...52(Vol 3)
heptanal...1(Vol 4)
heptane..155(Vol 1)
heptanoic acid..................................24(Vol 4)
1-heptanol..............1-heptyl alcohol......94(Vol 1)
1-heptene..165(Vol 1)

heptyl benzene..........189(Vol 3)
hexadecane..........129(Vol 3)
hexadecanoic acid..........44(Vol 4)
hexadecanol..........74(Vol 4)
hexadecene..........149(Vol 3)
hexafluoroethane........fluorocarbon-116......225(Vol 1)
hexamethylene glycol(1,6 hexanediol)..........164(Vol 4)
hexamethylenediamine..........184(Vol 4)
hexanal..........1(Vol 4)
hexane..........155(Vol 1)
hexanoic acid..........24(Vol 4)
1-hexanol..............1-hexyl alcohol.......94(Vol 1)
1-hexene..........165(Vol 1)
hexyl benzene..........179(Vol 3)
hexylene glycol(2 methyl 2,4 pentanediol)......164(Vol 4)
hydrogen..........52(Vol 3)
hydrogen bromide..........100(Vol 3)
hydrogen chloride..........100(Vol 3)
hydrogen cyanide..........126(Vol 2)
hydrogen fluoride..........100(Vol 3)
hydrogen iodide..........100(Vol 3)
hydrogen sulfide..........90(Vol 3)
iodine..........110(Vol 3)
isobutane..............2-methylpropane.......175(Vol 1)
isobutyl alcohol..........84(Vol 1)
isobutyl formate..........124(Vol 4)
isobutylene.............2-methylpropene.......175(Vol 1)
isooctane...............2,2,4-trimethylpentane.185(Vol 1)
isopentane..............2-methylbutane........175(Vol 1)
isoprene................2-methyl-1,3-butadiene.175(Vol 1)
isopropanol.............isopropyl alcohol.....84(Vol 1)
isopropyl acetate..........134(Vol 4)
isopropyl amine..........116(Vol 2)
methane..........1(Vol 1)
methanethiol..........206(Vol 2)
methanol..........74(Vol 1)
methyl acetate..........66(Vol 2)
methyl acetylene........propyne...............24(Vol 1)
methyl acrylate..........76(Vol 2)
methyl amine..........96(Vol 2)
methyl bromide..........235(Vol 1)
methyl sec-butyl ether..........104(Vol 4)
methyl tert-butyl ether..........104(Vol 4)
methyl butyl ketone..........94(Vol 4)
methyl chloride..........44(Vol 1)
methyl chloroform.......1,1,1-trichloroethane..195(Vol 1)
methyl cyclohexane..........169(Vol 3)
methyl cyclopentane..........159(Vol 3)
methyl ether..........46(Vol 2)

methyl ethyl ketone..........................36(Vol 2)
methyl formate...............................114(Vol 4)
methyl isobutyl ketone.......................94(Vol 4)
methyl isopropyl ketone......................84(Vol 4)
methyl methacrylate..........................76(Vol 2)
methyl propyl ketone.........................84(Vol 4)
methylene chloride......dichloromethane.......44(Vol 1)
n methylacetamide............................204(Vol 4)
n methylformamide............................194(Vol 4)
2-methylheptane..............................185(Vol 1)
2-methylhexane...............................185(Vol 1)
2-methylpentane.........isohexane.............185(Vol 1)
naphthelene..................................209(Vol 3)
neon...61(Vol 3)
nitrogen.....................................14(Vol 3)
nitrogen dioxide.............................70(Vol 3)
nitric oxide.................................70(Vol 3)
nitroethane..................................136(Vol 2)
nitromethane.................................136(Vol 2)
1-nitropropane...............................136(Vol 2)
2-nitropropane...............................136(Vol 2)
nitrous oxide................................70(Vol 3)
nonyl benzene................................189(Vol 3)
octadecane...................................129(Vol 3)
octadecanoic acid............................44(Vol 4)
octadecanol..................................74(Vol 4)
octadecene...................................149(Vol 3)
octanal......................................14(Vol 4)
octane.......................................155(Vol 1)
octanoic acid................................34(Vol 4)
octanol......................................64(Vol 4)
1-octene.....................................165(Vol 1)
octyl benzene................................189(Vol 3)
oxygen.......................................14(Vol 3)
ozone..32(Vol 3)
pentane......................................155(Vol 1)
pentanoic acid...............................24(Vol 4)
1-pentanol.............1-amyl alcohol.........94(Vol 1)
1-pentene..............isopentene.............165(Vol 1)
pentyl benzene...............................179(Vol 3)
perchloroethylene............................54(Vol 1)
phosgene.....................................16(Vol 2)
prionaldehyde................................6(Vol 2)
propadiene.............allene.................34(Vol 1)
propane......................................1(Vol 1)
propanol...............propyl alcohol.........74(Vol 1)
propionic acid...............................26(Vol 2)
propionic anhydride..........................86(Vol 2)
propionitrile................................126(Vol 2)

propyl acetate................................134(Vol 4)
propyl benzene.................................156(Vol 2)
propyl chloride.........1-chloropropane.......64(Vol 1)
propyl cyclohexane.............................169(Vol 3)
propyl cyclopentane............................159(Vol 3)
propyl ether....................................46(Vol 2)
propyl formate.................................114(Vol 4)
propylamine....................................174(Vol 4)
propylene..............propene...............14(Vol 1)
propylene dichloride.....1,2-dichloropropane....64(Vol 1)
propylene glycol........1,2-propylene glycol...135(Vol 1)
propylene oxide................................104(Vol 1)
pyridine.......................................146(Vol 2)
styrene..186(Vol 2)
succinic acid...................................54(Vol 4)
sulfur dioxide..................................80(Vol 3)
sulfur trioxide.................................80(Vol 3)
1,1,2,2-tertachloroethane......................195(Vol 1)
tetradecane....................................119(Vol 3)
tetradecanoic acid..............................44(Vol 4)
tetradecanol....................................74(Vol 4)
tetradecene....................................139(Vol 3)
tetrafluoromethane......fluorocarbon-14.......205(Vol 1)
tetrahydrofuran.................................56(Vol 2)
toluene..166(Vol 2)
trichloroethylene...............................54(Vol 1)
trichlorofluoromethane...fluorocarbon-11.......205(Vol 1)
1,1,2-trichloro-1,2,
 2-trifluoroethane......fluorocarbon-113.......215(Vol 1)
triethylamine..................................106(Vol 2)
triethylene gylcol.............................114(Vol 1)
trifluoromethane........fluorocarbon-23.......225(Vol 1)
trimethylamine..................................96(Vol 2)
tripropylamine.................................174(Vol 4)
undecyl benzene................................199(Vol 3)
vinyl acetate...................................66(Vol 2)
vinyl chloride..................................54(Vol 1)
vinyl fluoride.................................225(Vol 1)
vinylidene chloride.............................54(Vol 1)
vinylidene fluoride............................225(Vol 1)
m-xylene.......................................166(Vol 2)
o-xylene.......................................166(Vol 2)
p-xylene.......................................166(Vol 2)
water..216(Vol 2)

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About the Authors

Robert W. Gallant is vice-president and director of North America Operations for Dow Chemical Company, Midland, Michigan. He is the author of numerous technical articles and 4 books.

Carl L. Yaws, Ph.D., is a professor of chemical engineering at Lamar University, Beaumont, Texas. He is a registered professional engineer and the author of 17 books, including *Thermodynamic and Physical Property Data, Handbook of Transport Property Data, Handbook of Vapor Pressure* (4 volumes), *Handbook of Viscosity* (3 volumes), and *Handbook of Thermal Conductivity* (3 volumes). Mr. Gallant and he co-authored *Physical Properties of Hydrocarbons* (4 volumes).

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